



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 26, 2023 – 10:28 PM JST

PDB ID : 8KBW  
Title : The crystal structure of syn-copalyl diphosphate synthase from *Oryza sativa*  
Authors : Ma, X.L.; Xu, H.F.; Jiang, T.  
Deposited on : 2023-08-04  
Resolution : 3.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

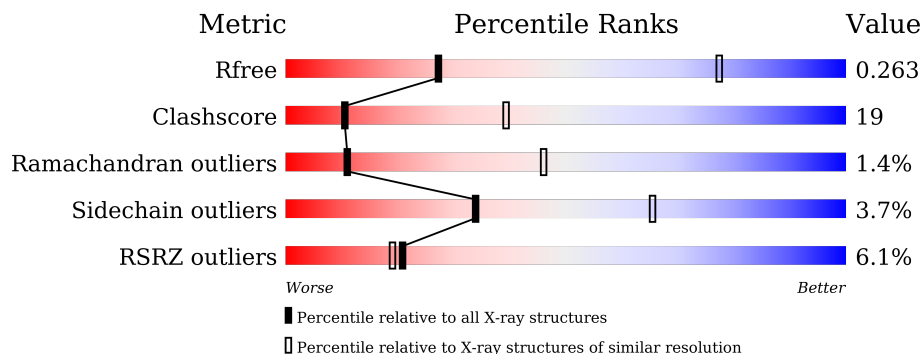
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	775	
1	B	775	
1	C	775	
1	D	775	
1	E	775	
1	F	775	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 32467 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Syn-copalyl diphosphate synthase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	668	5341	3391	916	1000	34	0	0	0
1	C	648	5186	3297	892	962	35	0	1	0
1	E	688	5504	3492	944	1033	35	0	0	0
1	D	688	5504	3492	944	1033	35	0	0	0
1	F	677	5421	3439	928	1019	35	0	0	0
1	A	689	5511	3496	945	1035	35	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

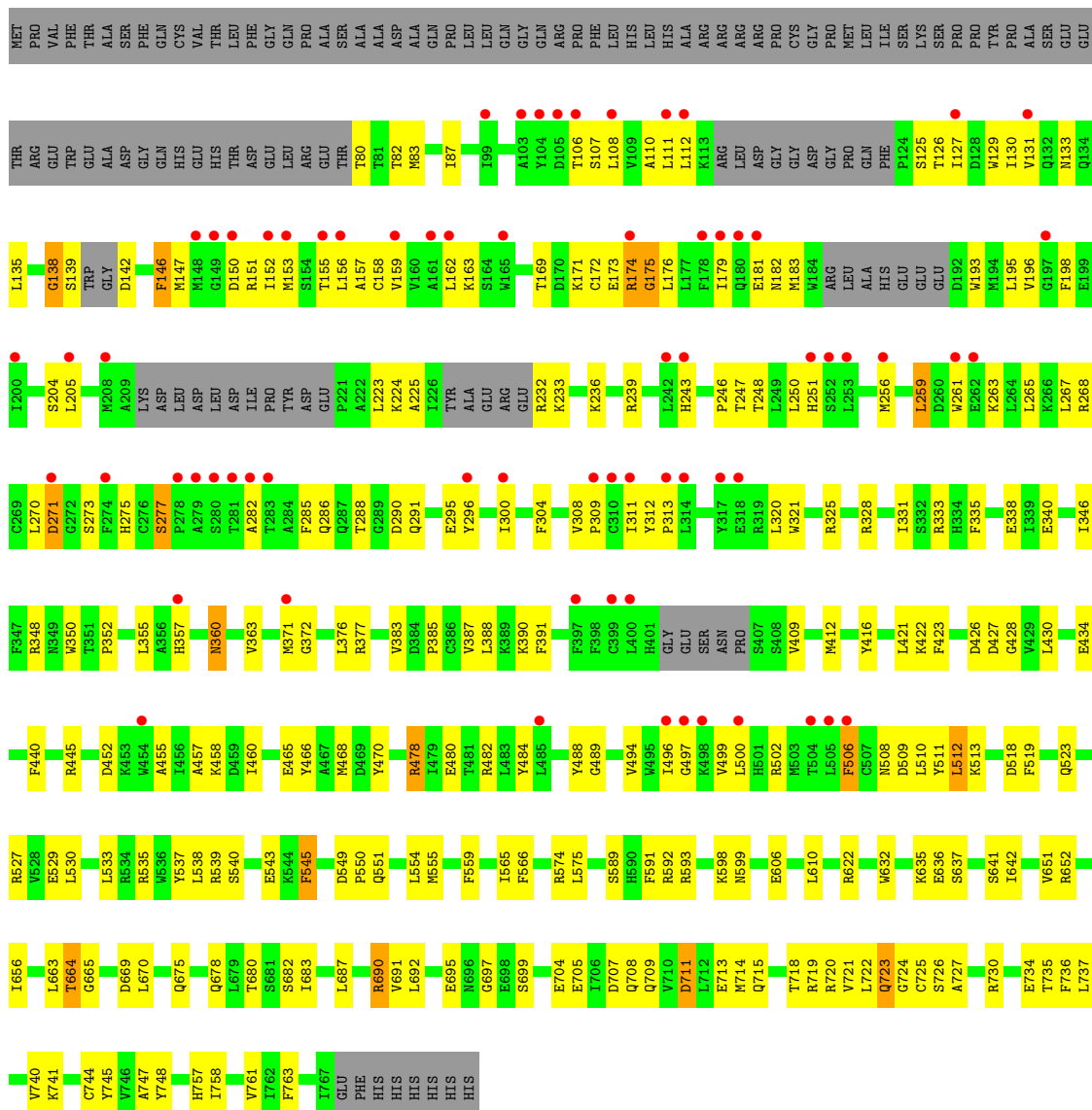
Chain	Residue	Modelled	Actual	Comment	Reference
B	768	GLU	-	expression tag	UNP Q0JF02
B	769	PHE	-	expression tag	UNP Q0JF02
B	770	HIS	-	expression tag	UNP Q0JF02
B	771	HIS	-	expression tag	UNP Q0JF02
B	772	HIS	-	expression tag	UNP Q0JF02
B	773	HIS	-	expression tag	UNP Q0JF02
B	774	HIS	-	expression tag	UNP Q0JF02
B	775	HIS	-	expression tag	UNP Q0JF02
C	768	GLU	-	expression tag	UNP Q0JF02
C	769	PHE	-	expression tag	UNP Q0JF02
C	770	HIS	-	expression tag	UNP Q0JF02
C	771	HIS	-	expression tag	UNP Q0JF02
C	772	HIS	-	expression tag	UNP Q0JF02
C	773	HIS	-	expression tag	UNP Q0JF02
C	774	HIS	-	expression tag	UNP Q0JF02
C	775	HIS	-	expression tag	UNP Q0JF02
E	768	GLU	-	expression tag	UNP Q0JF02

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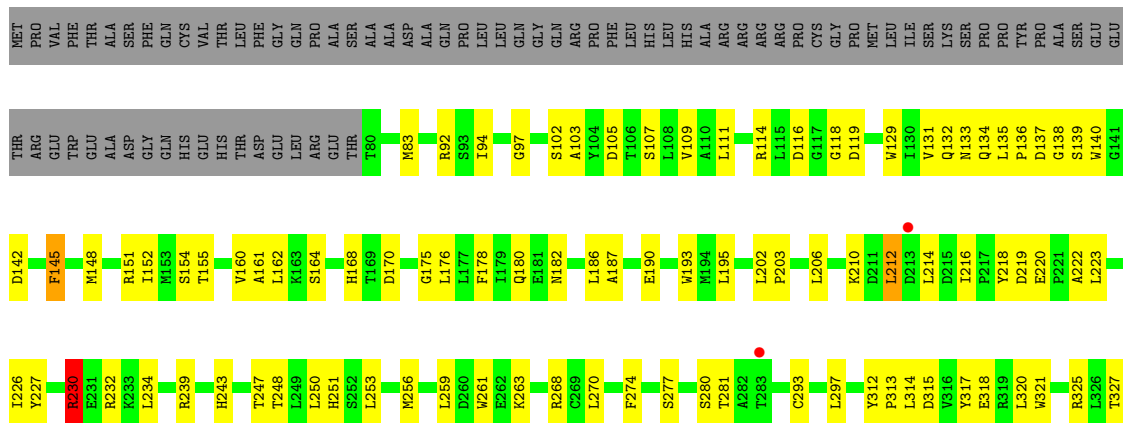
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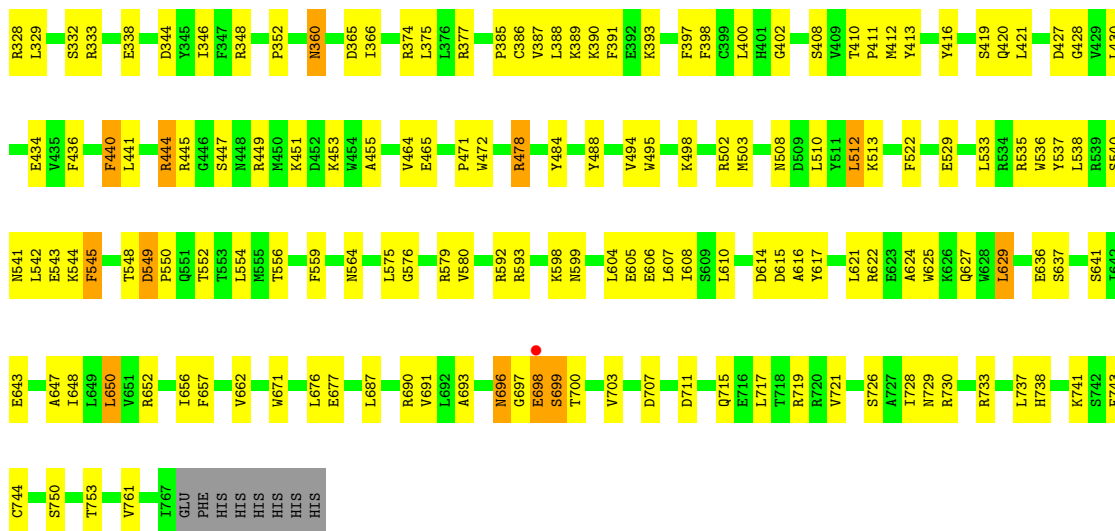
Chain	Residue	Modelled	Actual	Comment	Reference
E	769	PHE	-	expression tag	UNP Q0JF02
E	770	HIS	-	expression tag	UNP Q0JF02
E	771	HIS	-	expression tag	UNP Q0JF02
E	772	HIS	-	expression tag	UNP Q0JF02
E	773	HIS	-	expression tag	UNP Q0JF02
E	774	HIS	-	expression tag	UNP Q0JF02
E	775	HIS	-	expression tag	UNP Q0JF02
D	768	GLU	-	expression tag	UNP Q0JF02
D	769	PHE	-	expression tag	UNP Q0JF02
D	770	HIS	-	expression tag	UNP Q0JF02
D	771	HIS	-	expression tag	UNP Q0JF02
D	772	HIS	-	expression tag	UNP Q0JF02
D	773	HIS	-	expression tag	UNP Q0JF02
D	774	HIS	-	expression tag	UNP Q0JF02
D	775	HIS	-	expression tag	UNP Q0JF02
F	768	GLU	-	expression tag	UNP Q0JF02
F	769	PHE	-	expression tag	UNP Q0JF02
F	770	HIS	-	expression tag	UNP Q0JF02
F	771	HIS	-	expression tag	UNP Q0JF02
F	772	HIS	-	expression tag	UNP Q0JF02
F	773	HIS	-	expression tag	UNP Q0JF02
F	774	HIS	-	expression tag	UNP Q0JF02
F	775	HIS	-	expression tag	UNP Q0JF02
A	768	GLU	-	expression tag	UNP Q0JF02
A	769	PHE	-	expression tag	UNP Q0JF02
A	770	HIS	-	expression tag	UNP Q0JF02
A	771	HIS	-	expression tag	UNP Q0JF02
A	772	HIS	-	expression tag	UNP Q0JF02
A	773	HIS	-	expression tag	UNP Q0JF02
A	774	HIS	-	expression tag	UNP Q0JF02
A	775	HIS	-	expression tag	UNP Q0JF02



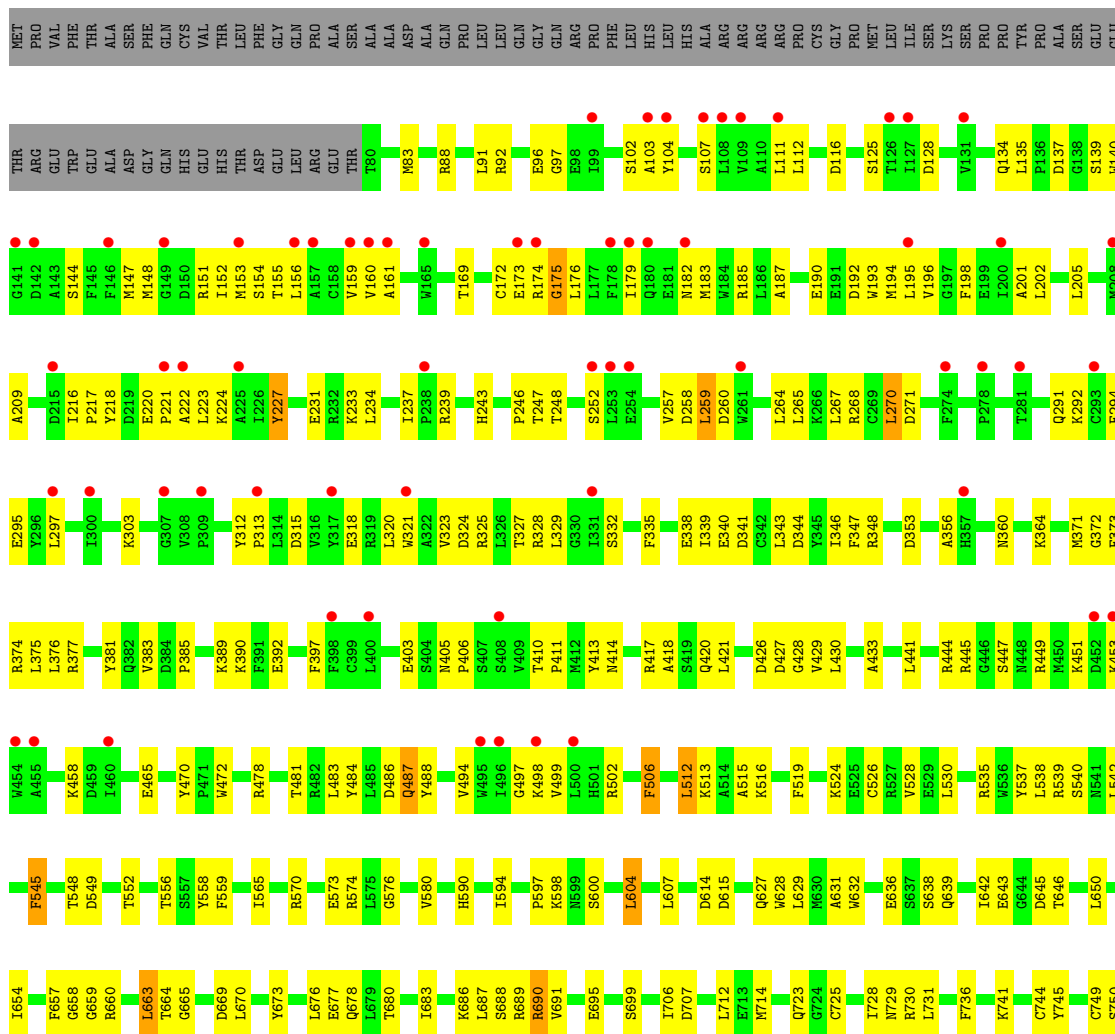


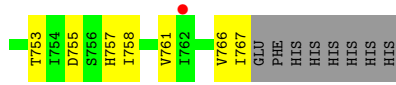
● Molecule 1: Syn-copalyl diphosphate synthase, chloroplatic



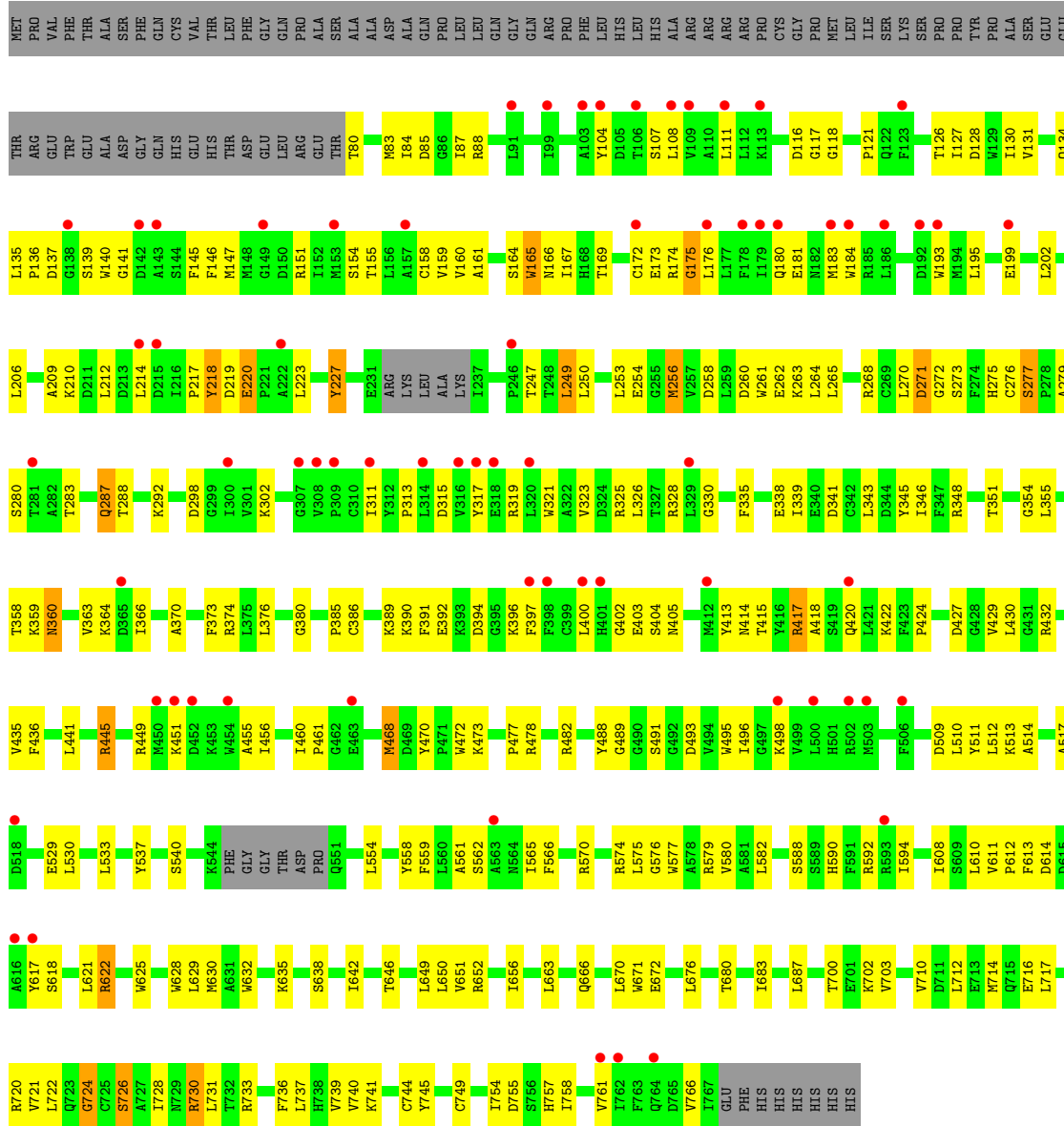


● Molecule 1: Syn-copalyl diphosphate synthase, chloroplastic

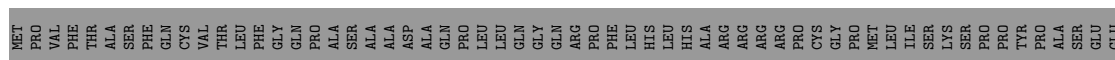




● Molecule 1: Syn-copalyl diphosphate synthase, chloroplastic



● Molecule 1: Syn-copalyl diphosphate synthase, chloroplastic





HIS	HIS	HIS	A693	Q694	F695	N696	G697	E698	S699	K702	E705	I706	Q709	V710	D711	L712	Q715	E716	R720	V721	L722	Q723	S726	A727	I728	L731	T732	R733	E734	T735	F736	L737	K741	C744	Y745	Y748	C749	S750	T753	I754	D755	S756	H757	I758	L767	GIJ	PHE	HIS	HIS	HIS	HIS								
L604	V494	K389	F294	P217	P218	Y219	E296	Y296	L297	V301	A222	L223	K302	K303	F304	N305	V308	Y312	F313	R319	L320	R321	T327	R328	H242	H243	R333	S244	G428	H334	F336	T336	S337	D341	D344	Y345	I346	F347	R348	L355	T358	K359	L270	D271	G272	S273	F274	P278	A279	S280	T281	A282	F285	T288	G289	D290	Q291	K292	C293
K498	E392	K393	D394	F397	E403	P411	K513	A514	E529	L530	L538	R539	S540	F545	G546	G547	D426	D427	G428	V429	L430	G431	R432	A433	E434	F440	R444	R445	G446	S447	N448	R449	N450	K451	D452	A455	I456	L460	P461	E465	Y466	Y470	G596	P597	K598	N599	N603												
L607	I608	S609	L610	V611	F612	D614	Y617	L621	R622	M625	K626	Q627	M628	M632	T633	W548	X634	X635	E636	L642	D645	T646	L649	L650	V651	R652	L656	V662	L663	T664	G665	Q666	R667	P668	L670	M671	E672	L676	E677	Q678	L687	R690	V691	L692															
HIS	HIS	HIS	A143	M147	M148	G149	A150	R151	I152	M153	S154	T155	H156	A157	C158	V159	V160	A161	L162	K163	S164	W165	M166	I167	H168	T169	C172	L177	G195	F178	I179	Q180	E181	M182	M183	W184	H185	L186	E189	E190	E191	D192	W193	E199	L202	P203	S204	L205	L206	A209	K210	Q134	L135	W140					
THR	ARG	GLU	TRP	GLU	ALA	ASP	GLY	GLN	HIS	HIS	HIS	THR	ASP	GLU	LEU	ARG	GLU	T79	T80	F81	T82	M83	I87	L91	I94	G95	E96	I99	S100	A103	Y104	D105	T106	S107	L108	L111	L112	K113	R114	G120	P121	D128	W129	I130	V131	Q132	N133	Q134	L135	W140									

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.70Å 174.34Å 296.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	97.62 – 3.49 98.19 – 3.49	Depositor EDS
% Data completeness (in resolution range)	96.5 (97.62-3.49) 95.4 (98.19-3.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 3.49Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.201 , 0.263 0.201 , 0.263	Depositor DCC
$R_{free}$ test set	2000 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.5	Xtrriage
Anisotropy	0.366	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	32467	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.63	0/5634	0.84	4/7625 (0.1%)
1	B	0.54	0/5455	0.74	1/7375 (0.0%)
1	C	0.54	0/5297	0.75	1/7155 (0.0%)
1	D	0.51	0/5627	0.70	1/7615 (0.0%)
1	E	0.57	2/5627 (0.0%)	0.77	4/7615 (0.1%)
1	F	0.49	0/5540	0.75	3/7496 (0.0%)
All	All	0.55	2/33180 (0.0%)	0.76	14/44881 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	744	CYS	CB-SG	-6.91	1.70	1.82
1	E	698	GLU	CB-CG	5.77	1.63	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	LEU	CA-CB-CG	6.72	130.76	115.30
1	E	234	LEU	CA-CB-CG	6.52	130.29	115.30
1	F	249	LEU	CA-CB-CG	6.07	129.27	115.30
1	E	629	LEU	CA-CB-CG	-6.05	101.38	115.30
1	F	530	LEU	CA-CB-CG	5.90	128.87	115.30
1	E	650	LEU	CA-CB-CG	-5.83	101.89	115.30
1	E	212	LEU	CA-CB-CG	5.70	128.41	115.30
1	F	575	LEU	CA-CB-CG	5.70	128.40	115.30
1	A	570	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	D	270	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	156	LEU	CB-CG-CD1	-5.17	102.21	111.00
1	A	649	LEU	CA-CB-CG	5.14	127.12	115.30
1	C	635	LYS	CD-CE-NZ	5.06	123.34	111.70
1	B	388	LEU	CB-CG-CD2	-5.03	102.44	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5511	0	5420	228	0
1	B	5341	0	5268	196	0
1	C	5186	0	5140	199	0
1	D	5504	0	5413	199	0
1	E	5504	0	5413	181	0
1	F	5421	0	5323	224	0
All	All	32467	0	31977	1193	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1193) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:608:ILE:HD11	1:E:621:LEU:HD22	1.34	1.08
1:A:156:LEU:HD11	1:A:205:LEU:HG	1.38	1.04
1:F:460:ILE:HG23	1:F:461:PRO:HD3	1.49	0.94
1:B:606:GLU:O	1:B:608:ILE:N	2.01	0.92
1:B:156:LEU:HD11	1:B:205:LEU:HG	1.52	0.91
1:F:270:LEU:HB2	1:F:360:ASN:HB2	1.51	0.91
1:A:690:ARG:HB3	1:A:706:ILE:HG21	1.53	0.91
1:E:212:LEU:HD12	1:E:214:LEU:HD23	1.53	0.90
1:F:608:ILE:HD11	1:F:622:ARG:HA	1.53	0.90
1:A:567:GLU:HB2	1:A:570:ARG:HG3	1.56	0.88
1:C:110:ALA:HB2	1:C:127:ILE:HD11	1.55	0.87
1:E:103:ALA:HB3	1:E:154:SER:HB2	1.55	0.87
1:F:140:TRP:HD1	1:F:155:THR:HA	1.38	0.86
1:B:261:TRP:NE1	1:B:287:GLN:HG2	1.91	0.85
1:D:628:TRP:HE1	1:D:646:THR:HG22	1.42	0.85
1:C:445:ARG:HE	1:C:468:MET:HE1	1.41	0.85
1:A:651:VAL:HG23	1:A:735:THR:HG22	1.58	0.84
1:B:261:TRP:HE1	1:B:287:GLN:HG2	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:TRP:HD1	1:E:155:THR:HG23	1.44	0.83
1:B:494:VAL:HG22	1:B:502:ARG:HE	1.44	0.80
1:C:243:HIS:HB3	1:C:263:LYS:HG3	1.62	0.80
1:E:606:GLU:OE1	1:E:622:ARG:NH2	2.14	0.80
1:C:416:TYR:HE1	1:C:434:GLU:HG3	1.47	0.80
1:F:716:GLU:OE1	1:F:720:ARG:NH1	2.15	0.80
1:C:545:PHE:HB3	1:C:593:ARG:HH12	1.45	0.80
1:B:559:PHE:HE1	1:B:761:VAL:HG11	1.47	0.79
1:B:696:ASN:O	1:B:698:GLU:N	2.15	0.79
1:A:597:PRO:HG3	1:A:633:THR:HG22	1.62	0.79
1:F:488:TYR:HD2	1:F:512:LEU:HG	1.48	0.79
1:A:389:LYS:HB3	1:A:429:VAL:HG11	1.65	0.79
1:E:134:GLN:HG2	1:E:140:TRP:CZ2	2.18	0.79
1:F:183:MET:HG3	1:F:220:GLU:HG2	1.63	0.78
1:C:466:TYR:HE1	1:C:470:TYR:HB2	1.47	0.77
1:F:330:GLY:HA3	1:F:478:ARG:HH12	1.50	0.77
1:E:248:THR:HG21	1:E:400:LEU:HD22	1.65	0.77
1:F:700:THR:HA	1:F:703:VAL:HG12	1.67	0.77
1:A:104:TYR:OH	1:A:254:GLU:HG3	1.85	0.77
1:B:270:LEU:HB3	1:B:360:ASN:HB2	1.65	0.77
1:A:750:SER:HB2	1:A:753:THR:HG23	1.66	0.76
1:A:597:PRO:HD2	1:A:636:GLU:OE2	1.84	0.76
1:B:614:ASP:HB3	1:B:617:TYR:HB2	1.67	0.76
1:B:429:VAL:HG12	1:B:432:ARG:NH2	2.01	0.76
1:F:261:TRP:HE1	1:F:287:GLN:HG2	1.51	0.76
1:E:540:SER:HB3	1:E:610:LEU:HD22	1.67	0.76
1:D:559:PHE:HE1	1:D:761:VAL:HG11	1.49	0.75
1:B:203:PRO:HG3	1:B:230:ARG:HG3	1.69	0.75
1:E:270:LEU:HB2	1:E:360:ASN:HB2	1.68	0.75
1:B:429:VAL:HG12	1:B:432:ARG:HH21	1.50	0.75
1:B:687:LEU:HD21	1:B:744:CYS:HA	1.69	0.74
1:B:540:SER:HB3	1:B:610:LEU:HD22	1.68	0.74
1:C:169:THR:HA	1:C:172:CYS:HB2	1.69	0.74
1:C:270:LEU:HB2	1:C:360:ASN:HB2	1.67	0.74
1:F:628:TRP:HE1	1:F:646:THR:HG22	1.49	0.74
1:E:243:HIS:HB3	1:E:263:LYS:HG3	1.70	0.74
1:B:445:ARG:HH11	1:B:465:GLU:HG3	1.51	0.74
1:A:716:GLU:OE2	1:A:720:ARG:NH1	2.20	0.73
1:E:542:LEU:HD11	1:E:610:LEU:HD13	1.68	0.73
1:B:220:GLU:HB3	1:B:223:LEU:HB2	1.71	0.73
1:C:466:TYR:CE1	1:C:470:TYR:HB2	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:648:ILE:HG12	1:E:677:GLU:HG2	1.69	0.73
1:C:250:LEU:HD21	1:C:267:LEU:HB3	1.69	0.73
1:A:529:GLU:HB3	1:A:575:LEU:HD21	1.69	0.73
1:D:140:TRP:CD1	1:D:155:THR:HA	2.23	0.73
1:E:317:TYR:HE2	1:E:503:MET:HE3	1.53	0.73
1:F:683:ILE:HD13	1:F:714:MET:HE2	1.70	0.73
1:E:129:TRP:O	1:E:133:ASN:ND2	2.19	0.72
1:D:196:VAL:HG22	1:D:497:GLY:C	2.08	0.72
1:F:396:LYS:HA	1:F:436:PHE:HE2	1.52	0.72
1:F:140:TRP:CD1	1:F:155:THR:HA	2.22	0.71
1:E:92:ARG:NH2	1:E:338:GLU:OE1	2.23	0.71
1:D:576:GLY:O	1:D:580:VAL:HG12	1.89	0.71
1:D:488:TYR:HD2	1:D:512:LEU:HG	1.54	0.71
1:C:135:LEU:HD21	1:C:139:SER:HB2	1.72	0.71
1:E:393:LYS:HB2	1:E:398:PHE:HE2	1.55	0.71
1:A:236:LYS:O	1:A:238:PRO:HD3	1.90	0.71
1:C:704:GLU:HA	1:C:707:ASP:HB2	1.72	0.71
1:D:103:ALA:HB3	1:D:154:SER:HB2	1.72	0.70
1:B:593:ARG:HB2	1:B:593:ARG:CZ	2.21	0.70
1:E:698:GLU:HG2	1:E:699:SER:H	1.56	0.70
1:D:628:TRP:NE1	1:D:646:THR:HG22	2.07	0.70
1:F:608:ILE:CD1	1:F:622:ARG:HA	2.22	0.69
1:C:540:SER:HB2	1:C:610:LEU:HD22	1.74	0.69
1:E:140:TRP:CD1	1:E:155:THR:HG23	2.28	0.69
1:D:565:ILE:HD11	1:D:570:ARG:HD3	1.75	0.69
1:F:389:LYS:HB3	1:F:429:VAL:HG11	1.75	0.69
1:D:194:MET:HG3	1:D:198:PHE:HD2	1.58	0.69
1:A:591:PHE:HE1	1:A:597:PRO:N	1.91	0.68
1:B:396:LYS:HA	1:B:436:PHE:CE2	2.28	0.68
1:C:108:LEU:HD23	1:C:282:ALA:HB3	1.76	0.68
1:D:140:TRP:HD1	1:D:155:THR:HG22	1.59	0.68
1:C:348:ARG:NH1	1:E:543:GLU:OE1	2.26	0.68
1:C:147:MET:O	1:C:151:ARG:HG2	1.94	0.68
1:C:664:THR:HG22	1:D:665:GLY:H	1.57	0.68
1:A:445:ARG:NH1	1:A:465:GLU:OE1	2.25	0.68
1:E:445:ARG:NH2	1:E:465:GLU:OE1	2.26	0.68
1:B:540:SER:HB2	1:B:542:LEU:HB2	1.75	0.68
1:D:231:GLU:HA	1:D:234:LEU:HG	1.76	0.68
1:D:683:ILE:HD13	1:D:714:MET:HE2	1.76	0.67
1:D:346:ILE:HG22	1:D:376:LEU:HD11	1.75	0.67
1:D:321:TRP:HB3	1:D:506:PHE:CZ	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:LYS:HB3	1:B:429:VAL:HG11	1.77	0.67
1:C:636:GLU:HG2	1:C:637:SER:H	1.58	0.67
1:B:680:THR:HG21	1:B:736:PHE:HD1	1.60	0.67
1:D:104:TYR:CD2	1:D:153:MET:HG2	2.30	0.67
1:E:719:ARG:NH2	1:F:630:MET:SD	2.68	0.67
1:B:696:ASN:OD1	1:B:697:GLY:N	2.27	0.66
1:F:268:ARG:HB2	1:F:273:SER:O	1.96	0.66
1:A:456:ILE:HD11	1:A:494:VAL:HB	1.78	0.66
1:F:385:PRO:HB2	1:F:430:LEU:HD13	1.77	0.66
1:D:169:THR:HA	1:D:172:CYS:HB2	1.77	0.66
1:F:651:VAL:HG12	1:F:739:VAL:HG21	1.76	0.66
1:F:351:THR:OG1	1:F:354:GLY:O	2.12	0.66
1:F:160:VAL:O	1:F:164:SER:HB2	1.97	0.65
1:A:130:ILE:O	1:A:140:TRP:HZ3	1.80	0.65
1:D:690:ARG:NH2	1:D:707:ASP:OD1	2.29	0.65
1:F:176:LEU:O	1:F:180:GLN:HG3	1.96	0.65
1:F:757:HIS:O	1:F:761:VAL:HG12	1.96	0.65
1:A:728:ILE:O	1:A:733:ARG:NH1	2.30	0.65
1:B:530:LEU:HD13	1:B:534:ARG:HH22	1.62	0.65
1:E:203:PRO:HB2	1:E:230:ARG:HD2	1.78	0.65
1:D:257:VAL:HG22	1:D:258:ASP:H	1.61	0.65
1:A:107:SER:O	1:A:111:LEU:HD22	1.96	0.65
1:D:413:TYR:CZ	1:D:417:ARG:HD2	2.31	0.65
1:D:321:TRP:HB3	1:D:506:PHE:CE1	2.31	0.65
1:B:195:LEU:HD13	1:B:196:VAL:H	1.62	0.64
1:B:195:LEU:HD13	1:B:196:VAL:N	2.12	0.64
1:A:238:PRO:HG2	1:A:241:VAL:HB	1.78	0.64
1:C:549:ASP:O	1:C:551:GLN:N	2.31	0.64
1:E:281:THR:HG23	1:E:293:CYS:SG	2.38	0.64
1:F:540:SER:HB2	1:F:610:LEU:HD22	1.79	0.64
1:B:603:ASN:O	1:B:603:ASN:ND2	2.30	0.64
1:F:83:MET:HG2	1:F:510:LEU:HD11	1.78	0.64
1:F:676:LEU:O	1:F:680:THR:HG23	1.97	0.64
1:E:559:PHE:HE1	1:E:761:VAL:HG11	1.63	0.64
1:E:408:SER:HB2	1:E:411:PRO:HD2	1.79	0.64
1:E:494:VAL:HG22	1:E:502:ARG:NH2	2.13	0.64
1:B:243:HIS:CD2	1:B:260:ASP:HB3	2.33	0.64
1:F:427:ASP:OD1	1:F:429:VAL:HG13	1.98	0.64
1:D:270:LEU:HB2	1:D:360:ASN:HB2	1.80	0.63
1:A:103:ALA:HB3	1:A:154:SER:HB2	1.79	0.63
1:B:116:ASP:N	1:B:116:ASP:OD1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:SER:HA	1:C:155:THR:HG23	1.81	0.63
1:B:554:LEU:HA	1:B:582:LEU:HD21	1.80	0.63
1:B:98:GLU:HB3	1:B:504:THR:HB	1.81	0.63
1:E:608:ILE:HD13	1:E:622:ARG:HA	1.80	0.63
1:F:721:VAL:HA	1:F:733:ARG:HG2	1.80	0.63
1:C:333:ARG:NH2	1:C:518:ASP:OD2	2.32	0.63
1:D:183:MET:HG3	1:D:220:GLU:HG3	1.80	0.63
1:D:542:LEU:HD13	1:D:542:LEU:O	1.97	0.63
1:B:393:LYS:HD2	1:B:398:PHE:CD2	2.34	0.63
1:C:340:GLU:OE2	1:E:535:ARG:NH2	2.32	0.63
1:C:181:GLU:OE2	1:C:182:ASN:ND2	2.32	0.63
1:C:664:THR:HG21	1:D:663:LEU:HD12	1.79	0.63
1:B:259:LEU:HD13	1:B:264:LEU:HD22	1.80	0.62
1:A:265:LEU:HD11	1:A:288:THR:HG21	1.81	0.62
1:D:243:HIS:CD2	1:D:260:ASP:HB3	2.33	0.62
1:E:627:GLN:OE1	1:F:720:ARG:NH2	2.32	0.62
1:D:420:GLN:HE21	1:D:420:GLN:HA	1.63	0.62
1:F:87:ILE:HD12	1:F:511:TYR:CD1	2.35	0.62
1:E:472:TRP:O	1:E:741:LYS:NZ	2.28	0.62
1:F:683:ILE:HD12	1:F:717:LEU:HD12	1.81	0.62
1:A:755:ASP:HA	1:A:758:ILE:HD12	1.81	0.62
1:B:673:TYR:CD1	1:A:670:LEU:HD21	2.34	0.62
1:A:411:PRO:O	1:A:415:THR:HG23	1.99	0.62
1:F:449:ARG:HA	1:F:451:LYS:HE2	1.82	0.62
1:A:604:LEU:HD22	1:A:607:LEU:HD22	1.80	0.62
1:E:145:PHE:HD2	1:E:494:VAL:HG21	1.64	0.62
1:B:243:HIS:HD2	1:B:260:ASP:HB3	1.64	0.62
1:A:608:ILE:HD11	1:A:625:TRP:CD1	2.35	0.62
1:A:270:LEU:HB2	1:A:360:ASN:HB2	1.82	0.61
1:A:204:SER:HB2	1:A:255:GLY:HA3	1.82	0.61
1:A:613:PHE:CE1	1:A:617:TYR:HB3	2.35	0.61
1:C:138:GLY:O	1:C:139:SER:OG	2.18	0.61
1:E:176:LEU:O	1:E:180:GLN:HG3	2.00	0.61
1:B:103:ALA:HB3	1:B:154:SER:HB2	1.81	0.61
1:B:242:LEU:HD12	1:B:249:LEU:HD23	1.80	0.61
1:B:473:LYS:NZ	1:B:711:ASP:OD2	2.23	0.61
1:C:107:SER:O	1:C:110:ALA:N	2.32	0.61
1:C:335:PHE:HB3	1:C:338:GLU:HB2	1.81	0.61
1:A:149:GLY:N	1:A:189:GLU:OE2	2.25	0.61
1:E:137:ASP:OD2	1:E:151:ARG:NH1	2.34	0.61
1:F:730:ARG:HG2	1:F:733:ARG:HH22	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:GLY:HA3	1:B:657:PHE:CE2	2.37	0.60
1:E:576:GLY:O	1:E:580:VAL:HG12	2.00	0.60
1:F:374:ARG:HG3	1:F:418:ALA:HA	1.83	0.60
1:B:204:SER:HB2	1:B:255:GLY:HA2	1.83	0.60
1:D:494:VAL:HG13	1:D:502:ARG:HG2	1.83	0.60
1:C:680:THR:HG21	1:C:736:PHE:HD1	1.65	0.60
1:F:611:VAL:HB	1:F:612:PRO:HD2	1.84	0.60
1:B:137:ASP:OD2	1:B:137:ASP:N	2.31	0.60
1:C:320:LEU:HD13	1:C:371:MET:HB3	1.83	0.60
1:C:458:LYS:HD3	1:C:489:GLY:HA2	1.83	0.60
1:C:535:ARG:HE	1:C:539[A]:ARG:NH1	1.99	0.60
1:E:698:GLU:CG	1:E:699:SER:H	2.14	0.60
1:F:628:TRP:NE1	1:F:646:THR:HG22	2.17	0.60
1:C:416:TYR:CE1	1:C:434:GLU:HG3	2.34	0.60
1:C:636:GLU:HG2	1:C:637:SER:N	2.16	0.60
1:F:728:ILE:HD11	1:F:733:ARG:HD3	1.84	0.60
1:A:140:TRP:CD1	1:A:155:THR:HA	2.37	0.60
1:E:320:LEU:HD21	1:E:346:ILE:HG12	1.82	0.60
1:C:445:ARG:NE	1:C:468:MET:HE1	2.15	0.59
1:C:535:ARG:HE	1:C:539[A]:ARG:HH12	1.49	0.59
1:F:217:PRO:O	1:F:219:ASP:N	2.35	0.59
1:F:396:LYS:HA	1:F:436:PHE:CE2	2.35	0.59
1:F:717:LEU:HD11	1:F:740:VAL:HG21	1.83	0.59
1:E:637:SER:HB3	1:F:712:LEU:HD11	1.83	0.59
1:D:628:TRP:HE1	1:D:646:THR:CG2	2.13	0.59
1:B:661:HIS:HD1	1:B:662:VAL:N	2.00	0.59
1:E:700:THR:O	1:E:703:VAL:N	2.36	0.59
1:E:537:TYR:CE2	1:E:543:GLU:HG2	2.37	0.59
1:F:374:ARG:HB2	1:F:418:ALA:HB2	1.85	0.59
1:A:663:LEU:O	1:A:664:THR:HG23	2.02	0.59
1:B:319:ARG:HD3	1:B:342:CYS:HB2	1.84	0.59
1:C:126:THR:O	1:C:130:ILE:HG13	2.02	0.59
1:E:160:VAL:O	1:E:164:SER:HB2	2.02	0.59
1:D:750:SER:O	1:D:753:THR:HG22	2.02	0.59
1:C:247:THR:H	1:C:250:LEU:HD13	1.68	0.59
1:F:223:LEU:O	1:F:227:TYR:HB2	2.02	0.59
1:A:83:MET:SD	1:A:513:LYS:HG2	2.43	0.59
1:C:321:TRP:HB3	1:C:506:PHE:CZ	2.37	0.59
1:F:121:PRO:N	1:F:165:TRP:HE1	2.00	0.59
1:B:608:ILE:HG13	1:B:609:SER:N	2.17	0.59
1:C:385:PRO:HB2	1:C:430:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:552:THR:O	1:E:556:THR:HG23	2.02	0.59
1:D:524:LYS:O	1:D:528:VAL:HG23	2.02	0.59
1:F:87:ILE:HG23	1:F:511:TYR:CE1	2.38	0.59
1:B:126:THR:O	1:B:130:ILE:HG13	2.02	0.58
1:B:488:TYR:HD2	1:B:512:LEU:HG	1.67	0.58
1:A:745:TYR:OH	1:A:757:HIS:ND1	2.28	0.58
1:A:413:TYR:CZ	1:A:417:ARG:HD3	2.38	0.58
1:F:195:LEU:HD23	1:F:496:ILE:HG23	1.85	0.58
1:A:140:TRP:HD1	1:A:155:THR:HG23	1.66	0.58
1:A:687:LEU:HD21	1:A:744:CYS:HA	1.85	0.58
1:C:664:THR:OG1	1:C:665:GLY:N	2.32	0.58
1:E:728:ILE:O	1:E:733:ARG:NH1	2.37	0.58
1:A:156:LEU:C	1:A:156:LEU:HD12	2.24	0.58
1:E:533:LEU:HD22	1:E:554:LEU:CD1	2.33	0.58
1:D:565:ILE:HD11	1:D:570:ARG:CD	2.33	0.58
1:A:255:GLY:O	1:A:256:MET:HG2	2.04	0.58
1:A:591:PHE:HE1	1:A:596:GLY:C	2.07	0.58
1:C:664:THR:HB	1:D:663:LEU:HA	1.84	0.58
1:E:206:LEU:HD13	1:E:223:LEU:HD21	1.85	0.58
1:A:183:MET:HG2	1:A:217:PRO:HG2	1.85	0.58
1:E:151:ARG:O	1:E:155:THR:OG1	2.19	0.58
1:D:104:TYR:HB3	1:D:499:VAL:HG21	1.84	0.58
1:F:147:MET:O	1:F:151:ARG:HG2	2.03	0.58
1:F:441:LEU:HB2	1:F:468:MET:CE	2.33	0.58
1:F:441:LEU:O	1:F:445:ARG:HB2	2.03	0.58
1:A:130:ILE:O	1:A:140:TRP:CZ3	2.56	0.58
1:A:148:MET:HG3	1:A:186:LEU:HD22	1.85	0.58
1:B:156:LEU:HD11	1:B:205:LEU:CG	2.32	0.57
1:B:281:THR:HG23	1:B:293:CYS:SG	2.44	0.57
1:C:488:TYR:HD2	1:C:512:LEU:HG	1.68	0.57
1:E:140:TRP:CD1	1:E:155:THR:HA	2.39	0.57
1:E:508:ASN:OD1	1:E:510:LEU:N	2.37	0.57
1:D:766:VAL:O	1:D:767:ILE:HG13	2.03	0.57
1:B:447:SER:HB3	1:B:449:ARG:HG3	1.86	0.57
1:E:447:SER:OG	1:E:449:ARG:NH1	2.37	0.57
1:E:604:LEU:HA	1:E:607:LEU:HD13	1.85	0.57
1:D:216:ILE:HG13	1:D:218:TYR:CE1	2.40	0.57
1:A:140:TRP:CD1	1:A:155:THR:HG23	2.39	0.57
1:A:579:ARG:HD2	1:A:611:VAL:HG13	1.86	0.57
1:E:693:ALA:HA	1:E:696:ASN:HB2	1.85	0.57
1:A:112:LEU:HD11	1:A:282:ALA:HB1	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:LEU:HD12	1:F:139:SER:H	1.69	0.57
1:F:253:LEU:HA	1:F:256:MET:HG2	1.85	0.57
1:E:138:GLY:O	1:E:175:GLY:HA2	2.05	0.57
1:C:722:LEU:O	1:C:724:GLY:N	2.37	0.57
1:E:397:PHE:HB2	1:E:436:PHE:CE2	2.40	0.57
1:D:259:LEU:H	1:D:259:LEU:HD23	1.68	0.57
1:F:155:THR:O	1:F:159:VAL:HG23	2.03	0.57
1:A:690:ARG:HB3	1:A:706:ILE:CG2	2.31	0.57
1:E:203:PRO:HB2	1:E:230:ARG:HH11	1.70	0.57
1:D:327:THR:HA	1:D:332:SER:HB3	1.87	0.57
1:F:429:VAL:HG12	1:F:432:ARG:HH21	1.69	0.57
1:C:175:GLY:O	1:C:179:ILE:HG13	2.05	0.57
1:E:447:SER:HB2	1:E:449:ARG:HG2	1.87	0.57
1:F:265:LEU:HD11	1:F:288:THR:HG21	1.86	0.57
1:D:134:GLN:HG3	1:D:140:TRP:CZ2	2.40	0.57
1:D:246:PRO:N	1:D:267:LEU:HD12	2.20	0.57
1:D:519:PHE:HZ	1:D:761:VAL:HG23	1.70	0.57
1:F:135:LEU:HD11	1:F:139:SER:HB2	1.84	0.57
1:A:169:THR:HA	1:A:172:CYS:HB2	1.87	0.57
1:E:187:ALA:HB2	1:E:222:ALA:HB2	1.87	0.56
1:E:385:PRO:HB2	1:E:430:LEU:HD13	1.87	0.56
1:A:220:GLU:HG3	1:A:222:ALA:H	1.70	0.56
1:C:545:PHE:HB3	1:C:593:ARG:NH1	2.17	0.56
1:C:273:SER:HB3	1:C:296:TYR:CZ	2.40	0.56
1:C:529:GLU:HB3	1:C:575:LEU:HD21	1.85	0.56
1:E:202:LEU:HD23	1:E:226:ILE:HD11	1.88	0.56
1:D:252:SER:HB3	1:D:498:LYS:HE2	1.87	0.56
1:F:413:TYR:CZ	1:F:417:ARG:HD2	2.39	0.56
1:A:321:TRP:HB3	1:A:506:PHE:CE2	2.41	0.56
1:C:376:LEU:HB3	1:C:383:VAL:HG21	1.85	0.56
1:C:155:THR:O	1:C:158:CYS:HB2	2.05	0.56
1:C:705:GLU:O	1:C:709:GLN:HG3	2.06	0.56
1:F:206:LEU:O	1:F:210:LYS:N	2.38	0.56
1:D:192:ASP:HB3	1:D:453:LYS:HG2	1.88	0.56
1:A:358:THR:HG23	1:A:360:ASN:H	1.70	0.56
1:A:570:ARG:HD2	1:A:573:GLU:OE1	2.06	0.56
1:B:269:CYS:HB3	1:B:360:ASN:O	2.06	0.56
1:B:565:ILE:O	1:B:574:ARG:HD3	2.06	0.56
1:B:597:PRO:HA	1:B:600:SER:HB3	1.87	0.56
1:A:268:ARG:NH2	1:A:290:ASP:OD2	2.39	0.56
1:B:373:PHE:HZ	1:B:377:ARG:HH21	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:604:LEU:HA	1:D:607:LEU:HD13	1.88	0.56
1:F:730:ARG:HG2	1:F:733:ARG:NH2	2.21	0.56
1:A:613:PHE:CE1	1:A:617:TYR:CB	2.88	0.56
1:D:196:VAL:HG22	1:D:498:LYS:N	2.22	0.55
1:D:385:PRO:HB2	1:D:430:LEU:HD13	1.88	0.55
1:F:183:MET:HG2	1:F:217:PRO:HG2	1.87	0.55
1:B:214:LEU:HD12	1:B:214:LEU:O	2.05	0.55
1:F:127:ILE:HG21	1:F:167:ILE:HD11	1.89	0.55
1:D:392:GLU:HG3	1:D:397:PHE:CE1	2.41	0.55
1:C:259:LEU:HD12	1:C:261:TRP:CZ2	2.41	0.55
1:F:554:LEU:HA	1:F:582:LEU:HD21	1.88	0.55
1:F:614:ASP:HB3	1:F:617:TYR:CZ	2.42	0.55
1:A:424:PRO:HD3	1:A:715:GLN:HB3	1.89	0.55
1:A:690:ARG:NH2	1:A:748:TYR:HE1	2.04	0.55
1:C:321:TRP:HB3	1:C:506:PHE:CE1	2.41	0.55
1:D:182:ASN:OD1	1:D:185:ARG:NH1	2.31	0.55
1:E:203:PRO:HG2	1:E:230:ARG:HH11	1.72	0.55
1:D:590:HIS:O	1:D:594:ILE:HG12	2.07	0.55
1:F:160:VAL:HG12	1:F:212:LEU:HD13	1.89	0.55
1:B:652:ARG:O	1:B:656:ILE:HG13	2.07	0.55
1:C:275:HIS:CD2	1:C:363:VAL:HG11	2.42	0.55
1:D:597:PRO:HA	1:D:600:SER:HB3	1.88	0.54
1:F:107:SER:HB2	1:F:161:ALA:HB2	1.88	0.54
1:F:279:ALA:HB3	1:F:498:LYS:HZ2	1.73	0.54
1:F:652:ARG:O	1:F:656:ILE:HG13	2.07	0.54
1:A:621:LEU:HD12	1:A:656:ILE:HD12	1.88	0.54
1:C:530:LEU:HD21	1:C:555:MET:SD	2.47	0.54
1:B:346:ILE:HG22	1:B:376:LEU:HD11	1.90	0.54
1:E:687:LEU:O	1:E:691:VAL:HG23	2.07	0.54
1:F:181:GLU:O	1:F:184:TRP:HD1	1.91	0.54
1:C:142:ASP:HB3	1:C:500:LEU:HB2	1.90	0.54
1:F:83:MET:SD	1:F:513:LYS:HG2	2.47	0.54
1:B:251:HIS:CE1	1:B:277:SER:HB2	2.42	0.54
1:F:565:ILE:O	1:F:574:ARG:HD3	2.07	0.54
1:A:159:VAL:HG13	1:A:172:CYS:SG	2.47	0.54
1:A:285:PHE:CE1	1:A:294:PHE:HB2	2.42	0.54
1:A:613:PHE:CZ	1:A:617:TYR:HB3	2.43	0.54
1:B:103:ALA:O	1:B:106:THR:HG22	2.08	0.54
1:B:445:ARG:NH1	1:B:465:GLU:HG3	2.22	0.54
1:E:420:GLN:HE21	1:E:420:GLN:HA	1.72	0.54
1:D:680:THR:HG21	1:D:736:PHE:HD1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:LEU:HD13	1:F:137:ASP:HB3	1.89	0.54
1:A:565:ILE:O	1:A:574:ARG:HD3	2.08	0.54
1:A:705:GLU:O	1:A:709:GLN:HG2	2.08	0.54
1:B:104:TYR:OH	1:B:254:GLU:OE2	2.22	0.54
1:B:648:ILE:HD11	1:B:677:GLU:HB3	1.90	0.54
1:D:179:ILE:O	1:D:183:MET:HB2	2.08	0.54
1:F:588:SER:O	1:F:592:ARG:HD3	2.07	0.54
1:C:687:LEU:HD11	1:C:744:CYS:HA	1.90	0.54
1:E:134:GLN:HG2	1:E:140:TRP:CH2	2.43	0.54
1:F:169:THR:HA	1:F:172:CYS:HB2	1.89	0.54
1:A:135:LEU:HD23	1:A:140:TRP:HA	1.90	0.54
1:A:254:GLU:OE1	1:A:498:LYS:NZ	2.41	0.54
1:E:397:PHE:HB2	1:E:436:PHE:CD2	2.43	0.53
1:E:647:ALA:HB2	1:E:743:PHE:HE2	1.72	0.53
1:D:353:ASP:OD1	1:D:390:LYS:HE2	2.08	0.53
1:F:173:GLU:C	1:F:175:GLY:H	2.12	0.53
1:A:392:GLU:OE1	1:A:432:ARG:NH2	2.41	0.53
1:C:711:ASP:O	1:C:715:GLN:HG3	2.08	0.53
1:A:706:ILE:O	1:A:710:VAL:HG12	2.08	0.53
1:B:239:ARG:NH2	1:B:258:ASP:O	2.40	0.53
1:B:420:GLN:HA	1:B:420:GLN:HE21	1.73	0.53
1:D:265:LEU:O	1:D:268:ARG:NH1	2.32	0.53
1:D:723:GLN:OE1	1:D:725:CYS:HB2	2.08	0.53
1:B:605:GLU:HA	1:B:629:LEU:HD11	1.90	0.53
1:B:721:VAL:HG11	1:B:737:LEU:HB2	1.90	0.53
1:C:606:GLU:OE2	1:C:622:ARG:NH1	2.36	0.53
1:F:617:TYR:HB3	1:F:656:ILE:HG22	1.89	0.53
1:A:148:MET:HE3	1:A:152:ILE:HG12	1.90	0.53
1:B:106:THR:HA	1:B:308:VAL:HG12	1.90	0.53
1:C:111:LEU:O	1:C:112:LEU:HD23	2.09	0.53
1:C:683:ILE:HD13	1:C:714:MET:HE2	1.89	0.53
1:C:690:ARG:NH2	1:C:707:ASP:OD2	2.42	0.53
1:D:691:VAL:O	1:D:695:GLU:HG2	2.07	0.53
1:F:146:PHE:CE1	1:F:151:ARG:HG3	2.43	0.53
1:A:460:ILE:HG23	1:A:461:PRO:HD3	1.90	0.53
1:B:396:LYS:HA	1:B:436:PHE:HE2	1.70	0.53
1:C:328:ARG:NH1	1:C:484:TYR:CZ	2.77	0.53
1:D:147:MET:O	1:D:151:ARG:HG2	2.08	0.53
1:F:646:THR:O	1:F:649:LEU:HB3	2.09	0.53
1:B:134:GLN:HG3	1:B:140:TRP:CE2	2.44	0.53
1:B:204:SER:CB	1:B:255:GLY:HA2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:MET:O	1:B:247:THR:HG23	2.09	0.53
1:C:691:VAL:HG11	1:C:747:ALA:HA	1.90	0.53
1:D:335:PHE:HB3	1:D:338:GLU:HG2	1.91	0.53
1:D:657:PHE:C	1:D:659:GLY:H	2.12	0.53
1:F:249:LEU:HD12	1:F:250:LEU:HD12	1.90	0.53
1:F:277:SER:OG	1:F:280:SER:HB2	2.07	0.53
1:C:153:MET:HE3	1:C:198:PHE:HE1	1.73	0.53
1:C:664:THR:HG22	1:D:665:GLY:N	2.24	0.53
1:D:156:LEU:O	1:D:160:VAL:HG22	2.09	0.53
1:A:156:LEU:O	1:A:160:VAL:HG22	2.08	0.53
1:A:302:LYS:HG3	1:A:303:LYS:N	2.24	0.53
1:B:209:ALA:HA	1:B:214:LEU:HD21	1.90	0.53
1:F:386:CYS:O	1:F:389:LYS:HG2	2.08	0.53
1:F:146:PHE:HE1	1:F:151:ARG:HG3	1.74	0.53
1:F:261:TRP:NE1	1:F:287:GLN:HG2	2.21	0.53
1:F:730:ARG:HA	1:F:733:ARG:NH1	2.23	0.53
1:A:193:TRP:CZ3	1:A:456:ILE:HG22	2.43	0.53
1:A:690:ARG:O	1:A:694:GLN:N	2.42	0.53
1:C:589:SER:HA	1:C:592:ARG:HE	1.74	0.52
1:E:488:TYR:HD2	1:E:512:LEU:HG	1.73	0.52
1:E:717:LEU:O	1:E:721:VAL:HG23	2.09	0.52
1:D:673:TYR:CE1	1:D:677:GLU:HG3	2.44	0.52
1:A:134:GLN:HG3	1:A:140:TRP:CZ2	2.45	0.52
1:A:319:ARG:CD	1:A:345:TYR:HD2	2.21	0.52
1:C:745:TYR:OH	1:C:757:HIS:ND1	2.33	0.52
1:E:190:GLU:HG3	1:E:193:TRP:HE3	1.73	0.52
1:D:247:THR:OG1	1:D:248:THR:N	2.42	0.52
1:F:116:ASP:O	1:F:118:GLY:N	2.41	0.52
1:B:149:GLY:O	1:B:153:MET:HB3	2.09	0.52
1:B:651:VAL:HG12	1:B:739:VAL:HG21	1.92	0.52
1:D:650:LEU:O	1:D:654:ILE:HG13	2.09	0.52
1:F:271:ASP:OD2	1:F:313:PRO:HD3	2.09	0.52
1:A:530:LEU:HD11	1:A:555:MET:SD	2.50	0.52
1:A:587:VAL:O	1:A:591:PHE:HB2	2.08	0.52
1:A:672:GLU:OE2	1:A:726:SER:HB2	2.08	0.52
1:B:88:ARG:HG2	1:B:335:PHE:CD1	2.44	0.52
1:C:527:ARG:HH21	1:C:763:PHE:HA	1.73	0.52
1:F:84:ILE:HG23	1:F:335:PHE:HE1	1.75	0.52
1:F:265:LEU:O	1:F:268:ARG:NH1	2.43	0.52
1:B:268:ARG:HD2	1:B:272:GLY:O	2.09	0.52
1:E:608:ILE:HD12	1:E:625:TRP:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:726:SER:HB3	1:E:733:ARG:NH1	2.24	0.52
1:F:183:MET:CE	1:F:223:LEU:HD11	2.39	0.52
1:A:134:GLN:HG3	1:A:140:TRP:CE2	2.45	0.52
1:B:220:GLU:HG3	1:B:222:ALA:H	1.75	0.52
1:B:377:ARG:HG3	1:B:377:ARG:HH11	1.74	0.52
1:B:538:LEU:C	1:B:540:SER:H	2.13	0.52
1:E:277:SER:HB3	1:E:280:SER:HB2	1.91	0.52
1:F:529:GLU:OE1	1:F:574:ARG:NH2	2.36	0.52
1:D:757:HIS:O	1:D:761:VAL:HG12	2.10	0.52
1:F:141:GLY:N	1:F:154:SER:OG	2.42	0.52
1:F:358:THR:HG23	1:F:360:ASN:H	1.74	0.52
1:F:559:PHE:CE1	1:F:761:VAL:HG11	2.45	0.52
1:A:179:ILE:O	1:A:183:MET:HB2	2.08	0.52
1:D:636:GLU:C	1:D:638:SER:H	2.14	0.52
1:B:268:ARG:NH1	1:B:293:CYS:HB2	2.25	0.51
1:C:173:GLU:C	1:C:175:GLY:H	2.13	0.51
1:C:273:SER:HB3	1:C:296:TYR:CE1	2.43	0.51
1:C:409:VAL:HA	1:C:440:PHE:HE2	1.74	0.51
1:E:393:LYS:HB2	1:E:398:PHE:CE2	2.40	0.51
1:D:202:LEU:HD12	1:D:205:LEU:HB3	1.92	0.51
1:A:320:LEU:HG	1:A:346:ILE:CD1	2.40	0.51
1:A:597:PRO:CG	1:A:633:THR:HG22	2.37	0.51
1:C:412:MET:HG3	1:C:440:PHE:CD2	2.46	0.51
1:E:327:THR:HA	1:E:332:SER:HB3	1.92	0.51
1:D:134:GLN:HG3	1:D:140:TRP:CE2	2.46	0.51
1:D:690:ARG:HB2	1:D:706:ILE:HG21	1.91	0.51
1:A:160:VAL:O	1:A:164:SER:HB2	2.10	0.51
1:A:302:LYS:NZ	1:A:303:LYS:HB3	2.25	0.51
1:B:146:PHE:CD1	1:B:151:ARG:HG3	2.45	0.51
1:B:427:ASP:OD1	1:B:429:VAL:HG13	2.10	0.51
1:B:549:ASP:OD1	1:B:549:ASP:N	2.44	0.51
1:D:270:LEU:HB2	1:D:360:ASN:CB	2.40	0.51
1:A:380:GLY:HA2	1:A:722:LEU:O	2.10	0.51
1:C:669:ASP:OD1	1:C:727:ALA:HB3	2.11	0.51
1:E:420:GLN:OE1	1:E:471:PRO:HA	2.11	0.51
1:F:254:GLU:HA	1:F:283:THR:HG21	1.92	0.51
1:A:209:ALA:HB1	1:A:214:LEU:HD12	1.91	0.51
1:A:613:PHE:CD2	1:A:621:LEU:HD22	2.45	0.51
1:B:202:LEU:N	1:B:203:PRO:HD2	2.25	0.51
1:C:87:ILE:HD11	1:C:511:TYR:CD1	2.45	0.51
1:E:598:LYS:HG3	1:E:636:GLU:OE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:ASP:OD2	1:D:328:ARG:NH2	2.28	0.51
1:D:598:LYS:HG2	1:D:636:GLU:OE2	2.10	0.51
1:F:135:LEU:CD1	1:F:139:SER:H	2.24	0.51
1:F:253:LEU:HD12	1:F:256:MET:HG3	1.92	0.51
1:F:380:GLY:HA2	1:F:722:LEU:O	2.11	0.51
1:C:682:SER:HB3	1:C:713:GLU:OE1	2.11	0.51
1:C:737:LEU:HG	1:C:741:LYS:HD2	1.93	0.51
1:D:173:GLU:C	1:D:175:GLY:H	2.14	0.51
1:D:414:ASN:OD1	1:D:417:ARG:NH1	2.44	0.51
1:E:445:ARG:HD2	1:E:465:GLU:OE2	2.10	0.51
1:F:134:GLN:HG3	1:F:140:TRP:CZ2	2.46	0.51
1:F:173:GLU:O	1:F:175:GLY:N	2.44	0.51
1:A:79:THR:HG23	1:A:82:THR:H	1.75	0.51
1:D:545:PHE:CD2	1:D:590:HIS:HB2	2.46	0.51
1:A:265:LEU:HD22	1:A:268:ARG:CZ	2.40	0.51
1:B:525:GLU:O	1:B:529:GLU:HB2	2.11	0.51
1:E:216:ILE:HG13	1:E:218:TYR:CE2	2.45	0.51
1:E:251:HIS:CE1	1:E:277:SER:HB2	2.45	0.51
1:D:347:PHE:CD1	1:D:381:TYR:HD2	2.28	0.51
1:A:147:MET:O	1:A:151:ARG:HG2	2.11	0.51
1:A:259:LEU:HD12	1:A:259:LEU:O	2.11	0.51
1:C:152:ILE:HG12	1:C:156:LEU:HD23	1.93	0.50
1:E:440:PHE:CD1	1:E:440:PHE:C	2.84	0.50
1:F:565:ILE:HD13	1:F:570:ARG:CZ	2.42	0.50
1:A:737:LEU:HG	1:A:741:LYS:HD2	1.93	0.50
1:B:112:LEU:HD11	1:B:282:ALA:HB1	1.92	0.50
1:B:176:LEU:HA	1:B:179:ILE:HD12	1.92	0.50
1:C:390:LYS:C	1:C:391:PHE:HD1	2.15	0.50
1:C:565:ILE:O	1:C:574:ARG:HD3	2.12	0.50
1:C:652:ARG:O	1:C:656:ILE:HG13	2.11	0.50
1:E:508:ASN:OD1	1:E:510:LEU:HB3	2.11	0.50
1:D:329:LEU:HD23	1:D:515:ALA:HB2	1.93	0.50
1:F:321:TRP:O	1:F:325:ARG:HG2	2.11	0.50
1:C:247:THR:OG1	1:C:248:THR:N	2.45	0.50
1:C:720:ARG:NH2	1:D:627:GLN:OE1	2.42	0.50
1:D:88:ARG:HD3	1:D:92:ARG:NH2	2.27	0.50
1:F:135:LEU:HG	1:F:139:SER:O	2.11	0.50
1:B:115:LEU:HD23	1:E:116:ASP:HB3	1.94	0.50
1:E:162:LEU:HD22	1:E:168:HIS:HB2	1.92	0.50
1:D:193:TRP:CZ2	1:D:451:LYS:HD2	2.47	0.50
1:F:559:PHE:HE1	1:F:761:VAL:HG11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LEU:HA	1:A:111:LEU:HD23	1.92	0.50
1:A:333:ARG:HG3	1:A:334:HIS:HD2	1.76	0.50
1:A:613:PHE:CE2	1:A:621:LEU:HD22	2.47	0.50
1:B:214:LEU:O	1:B:216:ILE:HG12	2.12	0.50
1:F:579:ARG:NH1	1:F:612:PRO:HD3	2.27	0.50
1:F:724:GLY:HA2	1:F:733:ARG:NH2	2.26	0.50
1:A:268:ARG:HB2	1:A:273:SER:O	2.11	0.50
1:B:397:PHE:CE2	1:B:433:ALA:HA	2.47	0.50
1:A:668:PRO:HA	1:A:671:TRP:CE3	2.47	0.50
1:B:377:ARG:HD3	1:B:423:PHE:CZ	2.47	0.50
1:A:270:LEU:HB2	1:A:360:ASN:CB	2.41	0.50
1:B:91:LEU:HD21	1:B:326:LEU:HD11	1.94	0.50
1:B:535:ARG:NH2	1:D:340:GLU:OE1	2.44	0.50
1:B:605:GLU:HA	1:B:629:LEU:CD1	2.41	0.50
1:D:220:GLU:OE1	1:D:221:PRO:HD2	2.12	0.50
1:F:373:PHE:CZ	1:F:385:PRO:HB3	2.46	0.50
1:B:106:THR:OG1	1:B:307:GLY:HA2	2.12	0.49
1:B:427:ASP:OD1	1:B:428:GLY:N	2.45	0.49
1:E:377:ARG:HD3	1:E:421:LEU:HB3	1.94	0.49
1:E:533:LEU:HD22	1:E:554:LEU:HD13	1.94	0.49
1:D:270:LEU:HD22	1:D:360:ASN:HB3	1.93	0.49
1:D:687:LEU:HD21	1:D:744:CYS:HA	1.94	0.49
1:F:441:LEU:HB2	1:F:468:MET:HE1	1.93	0.49
1:B:377:ARG:HD2	1:B:421:LEU:HB3	1.94	0.49
1:B:682:SER:O	1:B:686:LYS:HD3	2.12	0.49
1:C:311:ILE:HD11	1:C:357:HIS:NE2	2.27	0.49
1:A:206:LEU:HG	1:A:218:TYR:HD2	1.77	0.49
1:C:651:VAL:HG23	1:C:735:THR:HG22	1.94	0.49
1:E:608:ILE:CD1	1:E:621:LEU:HD22	2.25	0.49
1:F:562:SER:HA	1:F:574:ARG:HD2	1.95	0.49
1:F:680:THR:HG21	1:F:736:PHE:HD1	1.76	0.49
1:C:320:LEU:HD21	1:C:372:GLY:HA2	1.93	0.49
1:E:729:ASN:OD1	1:E:730:ARG:N	2.44	0.49
1:B:131:VAL:HG13	1:B:132:GLN:HG3	1.93	0.49
1:B:482:ARG:HD3	1:B:519:PHE:CE1	2.48	0.49
1:E:320:LEU:CD2	1:E:346:ILE:HG12	2.43	0.49
1:E:536:TRP:CE2	1:E:579:ARG:HD3	2.48	0.49
1:D:530:LEU:HD21	1:D:558:TYR:CD1	2.47	0.49
1:B:569:ASN:C	1:B:571:ALA:H	2.16	0.49
1:C:246:PRO:HA	1:C:267:LEU:HD13	1.93	0.49
1:F:209:ALA:HB1	1:F:214:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:672:GLU:OE2	1:F:726:SER:HB2	2.12	0.49
1:A:206:LEU:HD13	1:A:227:TYR:OH	2.12	0.49
1:C:80:THR:N	1:C:82:THR:HG1	2.10	0.49
1:D:374:ARG:NH2	1:D:375:LEU:HD21	2.27	0.49
1:D:397:PHE:CE2	1:D:433:ALA:HA	2.48	0.49
1:D:565:ILE:O	1:D:574:ARG:HD3	2.13	0.49
1:A:386:CYS:O	1:A:389:LYS:HG2	2.11	0.49
1:A:597:PRO:HD2	1:A:636:GLU:CD	2.33	0.49
1:E:268:ARG:HB3	1:E:274:PHE:CE1	2.48	0.49
1:A:478:ARG:HD3	1:A:566:PHE:CG	2.48	0.49
1:A:666:GLN:N	1:A:666:GLN:OE1	2.46	0.49
1:B:460:ILE:HG22	1:B:461:PRO:HD3	1.95	0.49
1:E:247:THR:H	1:E:250:LEU:HD13	1.77	0.49
1:E:614:ASP:OD1	1:E:616:ALA:N	2.41	0.49
1:F:108:LEU:HA	1:F:111:LEU:HD12	1.93	0.49
1:A:635:LYS:NZ	1:A:645:ASP:OD2	2.45	0.49
1:B:134:GLN:HG3	1:B:140:TRP:CZ2	2.48	0.49
1:C:675:GLN:HG2	1:C:720:ARG:NH1	2.28	0.49
1:E:135:LEU:HB3	1:E:136:PRO:HD2	1.95	0.49
1:E:203:PRO:HG2	1:E:230:ARG:NH1	2.27	0.49
1:F:260:ASP:O	1:F:264:LEU:HB2	2.13	0.49
1:A:252:SER:HB3	1:A:498:LYS:HE2	1.94	0.49
1:A:597:PRO:CD	1:A:636:GLU:OE2	2.57	0.49
1:B:140:TRP:CD1	1:B:155:THR:HG23	2.48	0.48
1:E:83:MET:SD	1:E:513:LYS:HG2	2.53	0.48
1:E:393:LYS:HE2	1:E:402:GLY:H	1.77	0.48
1:A:333:ARG:HA	1:A:336:THR:HG23	1.95	0.48
1:D:410:THR:OG1	1:D:411:PRO:HD3	2.13	0.48
1:C:496:ILE:HD13	1:C:496:ILE:HA	1.65	0.48
1:E:416:TYR:HE1	1:E:434:GLU:HG3	1.78	0.48
1:D:155:THR:O	1:D:159:VAL:HG23	2.12	0.48
1:D:196:VAL:HG22	1:D:497:GLY:O	2.12	0.48
1:D:323:VAL:HG22	1:D:339:ILE:HG23	1.94	0.48
1:C:598:LYS:HB2	1:C:636:GLU:OE2	2.13	0.48
1:E:203:PRO:CG	1:E:230:ARG:HH11	2.25	0.48
1:D:389:LYS:HB3	1:D:429:VAL:HG11	1.96	0.48
1:D:413:TYR:HA	1:D:441:LEU:HD11	1.96	0.48
1:A:248:THR:HG23	1:A:403:GLU:OE2	2.13	0.48
1:A:613:PHE:HE1	1:A:617:TYR:CD2	2.31	0.48
1:C:135:LEU:HD21	1:C:151:ARG:HH22	1.78	0.48
1:C:683:ILE:O	1:C:687:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:SER:HA	1:B:430:LEU:HD11	1.96	0.48
1:B:538:LEU:O	1:B:540:SER:N	2.47	0.48
1:B:661:HIS:HD1	1:B:662:VAL:H	1.60	0.48
1:C:173:GLU:HG2	1:C:176:LEU:HD23	1.94	0.48
1:E:186:LEU:HA	1:E:186:LEU:HD23	1.63	0.48
1:E:564:ASN:HB3	1:E:738:HIS:ND1	2.29	0.48
1:B:233:LYS:O	1:B:237:ILE:HG23	2.12	0.48
1:B:628:TRP:HB2	1:B:649:LEU:HD13	1.94	0.48
1:C:107:SER:OG	1:C:157:ALA:HB1	2.13	0.48
1:C:704:GLU:O	1:C:708:GLN:NE2	2.43	0.48
1:F:417:ARG:HG2	1:F:417:ARG:HH11	1.77	0.48
1:A:163:LYS:NZ	1:A:169:THR:HB	2.29	0.48
1:B:259:LEU:HD11	1:B:261:TRP:CZ2	2.49	0.48
1:E:202:LEU:N	1:E:203:PRO:HD2	2.28	0.48
1:F:403:GLU:O	1:F:405:ASN:N	2.47	0.48
1:F:432:ARG:O	1:F:435:VAL:HG12	2.13	0.48
1:A:559:PHE:CE2	1:A:758:ILE:HA	2.49	0.48
1:C:112:LEU:HD21	1:C:286:GLN:HG3	1.96	0.48
1:C:265:LEU:HG	1:C:268:ARG:HD2	1.95	0.48
1:A:312:TYR:CG	1:A:313:PRO:HA	2.48	0.48
1:A:358:THR:HG23	1:A:360:ASN:N	2.29	0.48
1:C:559:PHE:CG	1:C:758:ILE:HG12	2.49	0.48
1:C:664:THR:HA	1:D:664:THR:OG1	2.14	0.48
1:F:217:PRO:C	1:F:219:ASP:H	2.17	0.48
1:F:370:ALA:HB1	1:F:415:THR:HA	1.95	0.48
1:F:390:LYS:C	1:F:391:PHE:HD1	2.18	0.48
1:A:210:LYS:HB2	1:A:210:LYS:HE3	1.64	0.48
1:C:153:MET:HA	1:C:156:LEU:HG	1.95	0.47
1:E:711:ASP:O	1:E:715:GLN:HG3	2.14	0.47
1:D:135:LEU:CD1	1:D:137:ASP:HB3	2.44	0.47
1:D:140:TRP:CD1	1:D:155:THR:HG22	2.45	0.47
1:D:374:ARG:HG3	1:D:418:ALA:HA	1.95	0.47
1:C:663:LEU:HD22	1:C:663:LEU:H	1.79	0.47
1:E:494:VAL:HG22	1:E:502:ARG:CZ	2.44	0.47
1:A:273:SER:HB3	1:A:296:TYR:CZ	2.49	0.47
1:B:270:LEU:HB3	1:B:360:ASN:CB	2.39	0.47
1:E:416:TYR:CE1	1:E:434:GLU:HG3	2.49	0.47
1:E:652:ARG:O	1:E:656:ILE:HG13	2.14	0.47
1:F:424:PRO:HG3	1:F:716:GLU:HB2	1.96	0.47
1:F:635:LYS:O	1:F:638:SER:OG	2.28	0.47
1:A:449:ARG:O	1:A:450:MET:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:TRP:NE1	1:C:133:ASN:ND2	2.62	0.47
1:F:491:SER:OG	1:F:509:ASP:OD2	2.29	0.47
1:F:537:TYR:CD2	1:F:554:LEU:HD22	2.49	0.47
1:C:171:LYS:HA	1:C:174:ARG:HD3	1.95	0.47
1:E:139:SER:HB3	1:E:178:PHE:CD2	2.49	0.47
1:E:390:LYS:C	1:E:391:PHE:HD1	2.18	0.47
1:D:540:SER:OG	1:D:542:LEU:HB2	2.15	0.47
1:F:298:ASP:OD2	1:F:302:LYS:HD2	2.14	0.47
1:F:441:LEU:HB2	1:F:468:MET:HE3	1.97	0.47
1:B:111:LEU:HD21	1:B:161:ALA:HA	1.97	0.47
1:B:373:PHE:HZ	1:B:377:ARG:NH2	2.13	0.47
1:C:131:VAL:CG2	1:C:162:LEU:HD21	2.45	0.47
1:C:173:GLU:O	1:C:175:GLY:N	2.47	0.47
1:C:246:PRO:HD3	1:C:267:LEU:HD22	1.97	0.47
1:C:670:LEU:HD21	1:D:673:TYR:CD1	2.49	0.47
1:E:647:ALA:HB2	1:E:743:PHE:CE2	2.49	0.47
1:F:247:THR:HG23	1:F:249:LEU:HG	1.97	0.47
1:A:205:LEU:HD12	1:A:205:LEU:HA	1.52	0.47
1:A:328:ARG:NH1	1:A:484:TYR:CZ	2.83	0.47
1:A:591:PHE:CE1	1:A:597:PRO:HD3	2.50	0.47
1:B:458:LYS:HD3	1:B:489:GLY:HA2	1.97	0.47
1:C:256:MET:O	1:C:259:LEU:HD22	2.15	0.47
1:C:445:ARG:NH1	1:C:465:GLU:OE1	2.48	0.47
1:E:203:PRO:CB	1:E:230:ARG:HH11	2.27	0.47
1:D:148:MET:O	1:D:152:ILE:HG22	2.14	0.47
1:D:173:GLU:HA	1:D:176:LEU:HB3	1.96	0.47
1:A:427:ASP:OD1	1:A:428:GLY:N	2.47	0.47
1:B:750:SER:O	1:B:753:THR:HG22	2.14	0.47
1:C:265:LEU:HA	1:C:268:ARG:HD2	1.97	0.47
1:C:530:LEU:HD12	1:C:530:LEU:HA	1.60	0.47
1:E:344:ASP:HB3	1:E:348:ARG:HH12	1.79	0.47
1:E:455:ALA:HB2	1:E:495:TRP:CE3	2.50	0.47
1:E:545:PHE:HB3	1:E:593:ARG:NH2	2.29	0.47
1:D:483:LEU:O	1:D:487:GLN:HG2	2.15	0.47
1:D:538:LEU:HD12	1:F:348:ARG:NH1	2.30	0.47
1:F:755:ASP:HA	1:F:758:ILE:HD12	1.97	0.47
1:B:160:VAL:HG11	1:B:208:MET:HG2	1.97	0.46
1:B:300:ILE:HG21	1:B:308:VAL:HG21	1.96	0.46
1:B:661:HIS:ND1	1:B:662:VAL:N	2.64	0.46
1:C:478:ARG:NH1	1:C:566:PHE:CE2	2.83	0.46
1:F:537:TYR:HD2	1:F:554:LEU:HD22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:HIS:CD2	1:C:277:SER:HB3	2.50	0.46
1:C:271:ASP:O	1:C:296:TYR:HB2	2.14	0.46
1:C:722:LEU:HD12	1:C:722:LEU:N	2.31	0.46
1:D:209:ALA:O	1:D:218:TYR:OH	2.32	0.46
1:A:699:SER:CB	1:A:702:LYS:HB2	2.46	0.46
1:E:374:ARG:NH2	1:E:375:LEU:HD21	2.29	0.46
1:E:386:CYS:O	1:E:389:LYS:HG2	2.16	0.46
1:E:544:LYS:HG2	1:E:545:PHE:HD1	1.80	0.46
1:D:325:ARG:O	1:D:329:LEU:HD13	2.16	0.46
1:D:632:TRP:CD1	1:D:642:ILE:HD13	2.50	0.46
1:F:577:TRP:CD1	1:F:577:TRP:C	2.88	0.46
1:F:621:LEU:HD12	1:F:621:LEU:HA	1.74	0.46
1:F:642:ILE:O	1:F:646:THR:HG23	2.15	0.46
1:A:355:LEU:C	1:A:364:LYS:HD2	2.35	0.46
1:A:370:ALA:HB1	1:A:415:THR:HA	1.97	0.46
1:B:238:PRO:HG2	1:B:241:VAL:HB	1.97	0.46
1:C:152:ILE:HG23	1:C:153:MET:HE2	1.96	0.46
1:C:328:ARG:NH1	1:C:484:TYR:OH	2.49	0.46
1:F:328:ARG:HH21	1:F:417:ARG:NH1	2.13	0.46
1:A:363:VAL:O	1:A:363:VAL:HG13	2.14	0.46
1:A:483:LEU:HD23	1:A:483:LEU:HA	1.65	0.46
1:E:629:LEU:HD23	1:E:629:LEU:HA	1.72	0.46
1:D:107:SER:HB2	1:D:161:ALA:HB2	1.97	0.46
1:D:445:ARG:NH1	1:D:465:GLU:HG3	2.31	0.46
1:B:673:TYR:CE1	1:A:670:LEU:HD21	2.51	0.46
1:C:150:ASP:HB3	1:C:195:LEU:CD1	2.46	0.46
1:D:112:LEU:HD23	1:D:112:LEU:HA	1.67	0.46
1:D:356:ALA:N	1:D:364:LYS:HE3	2.30	0.46
1:F:87:ILE:HD12	1:F:511:TYR:CE1	2.51	0.46
1:F:687:LEU:HD21	1:F:744:CYS:HA	1.96	0.46
1:A:554:LEU:HA	1:A:582:LEU:HD21	1.97	0.46
1:F:323:VAL:HG22	1:F:339:ILE:HG23	1.98	0.46
1:F:403:GLU:OE1	1:F:405:ASN:ND2	2.49	0.46
1:B:214:LEU:O	1:B:214:LEU:CD1	2.64	0.46
1:B:656:ILE:HG12	1:A:667:ARG:CD	2.46	0.46
1:C:153:MET:HE2	1:C:153:MET:H	1.81	0.46
1:D:320:LEU:HD13	1:D:371:MET:HB3	1.98	0.46
1:F:85:ASP:HA	1:F:88:ARG:HB3	1.98	0.46
1:F:87:ILE:HD12	1:F:511:TYR:HD1	1.80	0.46
1:F:325:ARG:HA	1:F:325:ARG:HD3	1.80	0.46
1:A:642:ILE:O	1:A:645:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:709:GLN:O	1:B:709:GLN:HG2	2.16	0.46
1:C:265:LEU:HA	1:C:268:ARG:CD	2.46	0.46
1:C:457:ALA:HB3	1:C:460:ILE:HG12	1.98	0.46
1:E:107:SER:HB2	1:E:161:ALA:HB2	1.98	0.46
1:D:484:TYR:HA	1:D:487:GLN:CG	2.46	0.46
1:F:576:GLY:O	1:F:580:VAL:HG12	2.16	0.46
1:B:139:SER:HB3	1:B:178:PHE:CG	2.51	0.46
1:C:270:LEU:HB2	1:C:360:ASN:CB	2.44	0.46
1:E:152:ILE:HD13	1:E:152:ILE:HA	1.73	0.46
1:D:638:SER:OG	1:D:639:GLN:N	2.48	0.46
1:F:135:LEU:HD21	1:F:151:ARG:NH2	2.31	0.46
1:F:275:HIS:CD2	1:F:363:VAL:HG11	2.51	0.46
1:F:358:THR:HG23	1:F:360:ASN:N	2.31	0.46
1:F:455:ALA:HB2	1:F:495:TRP:CZ3	2.51	0.46
1:A:288:THR:HG22	1:A:290:ASP:HB2	1.98	0.46
1:A:320:LEU:HD23	1:A:320:LEU:HA	1.78	0.46
1:A:419:SER:HA	1:A:430:LEU:HD11	1.97	0.46
1:A:440:PHE:CD1	1:A:440:PHE:C	2.89	0.46
1:B:155:THR:O	1:B:159:VAL:HG23	2.16	0.45
1:E:721:VAL:HG11	1:E:737:LEU:HB2	1.97	0.45
1:D:83:MET:SD	1:D:513:LYS:HG2	2.56	0.45
1:D:686:LYS:HD2	1:D:689:ARG:NH2	2.30	0.45
1:F:127:ILE:O	1:F:131:VAL:HG13	2.16	0.45
1:F:214:LEU:HD12	1:F:218:TYR:OH	2.16	0.45
1:F:414:ASN:HA	1:F:417:ARG:HD3	1.98	0.45
1:B:146:PHE:HD1	1:B:151:ARG:HG3	1.82	0.45
1:B:214:LEU:HD13	1:B:216:ILE:HG12	1.97	0.45
1:B:410:THR:CG2	1:B:460:ILE:HD11	2.45	0.45
1:C:348:ARG:NH2	1:E:538:LEU:HD12	2.31	0.45
1:D:343:LEU:HD23	1:D:343:LEU:HA	1.52	0.45
1:F:565:ILE:HD11	1:F:570:ARG:HB3	1.98	0.45
1:F:608:ILE:HD13	1:F:625:TRP:HB3	1.97	0.45
1:F:629:LEU:O	1:F:632:TRP:HB2	2.16	0.45
1:A:663:LEU:HD22	1:A:663:LEU:H	1.81	0.45
1:B:292:LYS:HD2	1:B:292:LYS:HA	1.70	0.45
1:C:494:VAL:HG13	1:C:502:ARG:HG2	1.98	0.45
1:C:680:THR:HG22	1:C:740:VAL:HG21	1.98	0.45
1:F:151:ARG:O	1:F:155:THR:OG1	2.28	0.45
1:F:488:TYR:CD2	1:F:512:LEU:HG	2.39	0.45
1:A:319:ARG:HD2	1:A:345:TYR:HD2	1.81	0.45
1:E:139:SER:HB3	1:E:178:PHE:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:662:VAL:HG22	1:F:670:LEU:HD22	1.98	0.45
1:D:140:TRP:HD1	1:D:155:THR:HA	1.75	0.45
1:D:745:TYR:O	1:D:749:CYS:HB2	2.16	0.45
1:A:445:ARG:HD2	1:A:465:GLU:OE1	2.17	0.45
1:B:163:LYS:HG3	1:B:212:LEU:HD23	1.99	0.45
1:C:523:GLN:O	1:C:527:ARG:HG3	2.16	0.45
1:C:236:LYS:HB2	1:C:236:LYS:HE3	1.58	0.45
1:C:388:LEU:HD22	1:C:430:LEU:HD12	1.99	0.45
1:E:321:TRP:O	1:E:325:ARG:HG2	2.16	0.45
1:D:519:PHE:CZ	1:D:761:VAL:HG23	2.51	0.45
1:D:631:ALA:HB1	1:D:645:ASP:OD2	2.16	0.45
1:F:247:THR:HG23	1:F:250:LEU:HD13	1.97	0.45
1:F:650:LEU:HD23	1:F:650:LEU:HA	1.76	0.45
1:B:402:GLY:O	1:B:404:SER:N	2.50	0.45
1:C:721:VAL:HG11	1:C:737:LEU:HD22	1.98	0.45
1:D:195:LEU:HD13	1:D:498:LYS:O	2.17	0.45
1:D:325:ARG:HA	1:D:325:ARG:HD3	1.72	0.45
1:A:296:TYR:CD2	1:A:297:LEU:HD23	2.51	0.45
1:E:190:GLU:HB2	1:E:193:TRP:HB2	1.99	0.45
1:E:391:PHE:CD1	1:E:391:PHE:N	2.83	0.45
1:E:478:ARG:HG3	1:E:522:PHE:CZ	2.52	0.45
1:E:575:LEU:HD23	1:E:575:LEU:HA	1.83	0.45
1:D:614:ASP:OD1	1:D:615:ASP:N	2.50	0.45
1:F:128:ASP:O	1:F:131:VAL:HG22	2.16	0.45
1:F:489:GLY:HA3	1:F:493:ASP:OD1	2.17	0.45
1:B:519:PHE:HZ	1:B:761:VAL:HG23	1.82	0.45
1:C:159:VAL:HG13	1:C:172:CYS:SG	2.57	0.45
1:C:377:ARG:NH2	1:C:426:ASP:OD2	2.50	0.45
1:E:195:LEU:HD13	1:E:498:LYS:O	2.17	0.45
1:E:312:TYR:CG	1:E:313:PRO:HA	2.51	0.45
1:E:413:TYR:CD1	1:E:464:VAL:HG22	2.51	0.45
1:D:570:ARG:HH21	1:D:573:GLU:CD	2.21	0.45
1:F:326:LEU:HD22	1:F:335:PHE:HE2	1.82	0.45
1:A:731:LEU:HD13	1:A:731:LEU:HA	1.70	0.45
1:B:140:TRP:HD1	1:B:155:THR:HG23	1.81	0.45
1:C:533:LEU:HD23	1:C:554:LEU:HD11	1.99	0.45
1:C:545:PHE:CB	1:C:593:ARG:HH22	2.30	0.45
1:C:664:THR:CG2	1:D:663:LEU:HD12	2.47	0.45
1:F:104:TYR:O	1:F:108:LEU:HD12	2.17	0.45
1:F:554:LEU:HD13	1:F:582:LEU:HD11	1.99	0.45
1:A:692:LEU:HD23	1:A:692:LEU:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:THR:HA	1:C:172:CYS:CB	2.44	0.44
1:E:94:ILE:HD12	1:E:94:ILE:HA	1.69	0.44
1:E:131:VAL:HG11	1:E:168:HIS:CE1	2.51	0.44
1:E:606:GLU:CD	1:E:622:ARG:HH22	2.19	0.44
1:D:294:PHE:O	1:D:297:LEU:N	2.50	0.44
1:A:540:SER:HB2	1:A:610:LEU:HD22	1.99	0.44
1:C:391:PHE:CD1	1:C:391:PHE:N	2.85	0.44
1:E:427:ASP:OD1	1:E:428:GLY:N	2.50	0.44
1:D:104:TYR:OH	1:D:201:ALA:HB1	2.17	0.44
1:D:494:VAL:HG22	1:D:502:ARG:NE	2.32	0.44
1:A:87:ILE:O	1:A:91:LEU:HD23	2.18	0.44
1:C:482:ARG:HD3	1:C:519:PHE:CE1	2.52	0.44
1:C:499:VAL:HG12	1:C:500:LEU:N	2.31	0.44
1:E:529:GLU:HG2	1:E:575:LEU:HD11	1.98	0.44
1:E:537:TYR:CD2	1:E:543:GLU:HG2	2.52	0.44
1:E:608:ILE:HD12	1:E:625:TRP:HB2	1.98	0.44
1:F:420:GLN:HB3	1:F:472:TRP:HB2	1.99	0.44
1:F:533:LEU:HD13	1:F:554:LEU:HD11	1.99	0.44
1:F:651:VAL:HG12	1:F:739:VAL:CG2	2.46	0.44
1:A:114:ARG:HH12	1:A:120:GLY:H	1.66	0.44
1:A:193:TRP:CE3	1:A:456:ILE:HG22	2.52	0.44
1:B:575:LEU:HD23	1:B:575:LEU:HA	1.85	0.44
1:C:83:MET:HG2	1:C:510:LEU:HD11	2.00	0.44
1:D:629:LEU:O	1:D:632:TRP:HB2	2.17	0.44
1:F:319:ARG:HD2	1:F:345:TYR:HD2	1.82	0.44
1:F:355:LEU:C	1:F:364:LYS:HG3	2.38	0.44
1:A:203:PRO:HB2	1:A:230:ARG:NH2	2.33	0.44
1:A:494:VAL:HG22	1:A:502:ARG:CZ	2.47	0.44
1:C:156:LEU:HD11	1:C:205:LEU:CG	2.46	0.44
1:C:427:ASP:OD1	1:C:428:GLY:N	2.50	0.44
1:E:105:ASP:O	1:E:109:VAL:HG23	2.18	0.44
1:E:690:ARG:HD2	1:E:707:ASP:OD1	2.17	0.44
1:D:264:LEU:HA	1:D:267:LEU:HD23	2.00	0.44
1:D:328:ARG:O	1:D:481:THR:HG23	2.18	0.44
1:D:712:LEU:HD23	1:D:712:LEU:HA	1.73	0.44
1:F:400:LEU:HB2	1:F:403:GLU:HB3	2.00	0.44
1:A:80:THR:HA	1:A:83:MET:HE2	1.99	0.44
1:B:177:LEU:O	1:B:181:GLU:HG3	2.17	0.44
1:B:478:ARG:HD3	1:B:566:PHE:CG	2.53	0.44
1:E:388:LEU:HA	1:E:388:LEU:HD23	1.64	0.44
1:E:624:ALA:HB2	1:F:671:TRP:CH2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:526:CYS:O	1:D:530:LEU:HD23	2.18	0.44
1:F:206:LEU:HA	1:F:209:ALA:HB3	1.99	0.44
1:F:391:PHE:N	1:F:391:PHE:CD1	2.86	0.44
1:F:632:TRP:CD1	1:F:642:ILE:HD13	2.53	0.44
1:A:148:MET:CE	1:A:152:ILE:HG12	2.47	0.44
1:A:238:PRO:HG2	1:A:241:VAL:CB	2.45	0.44
1:B:216:ILE:O	1:B:218:TYR:N	2.51	0.44
1:E:317:TYR:CD1	1:E:321:TRP:CD1	3.06	0.44
1:F:199:GLU:CD	1:F:199:GLU:H	2.21	0.44
1:B:731:LEU:HA	1:B:731:LEU:HD23	1.66	0.44
1:C:466:TYR:HE2	1:C:480:GLU:CB	2.31	0.44
1:D:233:LYS:O	1:D:237:ILE:HG23	2.18	0.44
1:D:549:ASP:OD2	1:D:552:THR:OG1	2.35	0.44
1:F:608:ILE:HD13	1:F:625:TRP:CB	2.47	0.44
1:B:176:LEU:O	1:B:180:GLN:HG3	2.18	0.44
1:C:350:TRP:HA	1:C:355:LEU:HD21	1.98	0.44
1:E:366:ILE:HG22	1:E:411:PRO:HB3	1.99	0.44
1:A:106:THR:OG1	1:A:308:VAL:N	2.51	0.44
1:A:370:ALA:HB2	1:A:415:THR:HG22	2.00	0.44
1:A:456:ILE:HG12	1:A:494:VAL:O	2.17	0.44
1:C:146:PHE:HA	1:C:151:ARG:HD3	1.99	0.43
1:E:253:LEU:HA	1:E:253:LEU:HD23	1.85	0.43
1:E:410:THR:HB	1:E:411:PRO:HD3	2.00	0.43
1:F:590:HIS:O	1:F:594:ILE:HG12	2.17	0.43
1:A:397:PHE:CE2	1:A:433:ALA:HA	2.53	0.43
1:A:591:PHE:CE1	1:A:597:PRO:N	2.80	0.43
1:B:512:LEU:HD23	1:B:512:LEU:HA	1.46	0.43
1:E:148:MET:HE1	1:E:182:ASN:HB3	2.00	0.43
1:E:256:MET:HB3	1:E:259:LEU:CD2	2.48	0.43
1:E:313:PRO:O	1:E:314:LEU:HD23	2.17	0.43
1:E:559:PHE:CE1	1:E:761:VAL:HG11	2.50	0.43
1:F:145:PHE:HZ	1:F:193:TRP:CH2	2.36	0.43
1:F:209:ALA:HB1	1:F:214:LEU:HD21	2.00	0.43
1:A:227:TYR:O	1:A:230:ARG:HB3	2.18	0.43
1:A:341:ASP:O	1:A:344:ASP:HB2	2.19	0.43
1:B:130:ILE:O	1:B:140:TRP:HZ3	2.02	0.43
1:C:376:LEU:CB	1:C:383:VAL:HG21	2.47	0.43
1:C:690:ARG:HD2	1:C:748:TYR:HE1	1.84	0.43
1:D:643:GLU:HG3	1:D:688:SER:HB2	2.00	0.43
1:A:376:LEU:HA	1:A:376:LEU:HD23	1.76	0.43
1:A:652:ARG:O	1:A:656:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:ARG:HH21	1:B:555:MET:HE3	1.83	0.43
1:B:559:PHE:HE1	1:B:761:VAL:CG1	2.25	0.43
1:B:661:HIS:CD2	1:A:667:ARG:HG3	2.53	0.43
1:C:106:THR:HA	1:C:308:VAL:CG1	2.49	0.43
1:C:346:ILE:HG22	1:C:376:LEU:HD11	1.99	0.43
1:E:750:SER:HB2	1:E:753:THR:H	1.83	0.43
1:D:669:ASP:N	1:D:669:ASP:OD1	2.51	0.43
1:F:413:TYR:O	1:F:417:ARG:HD3	2.18	0.43
1:A:608:ILE:C	1:A:610:LEU:N	2.72	0.43
1:B:343:LEU:HD23	1:B:343:LEU:HA	1.74	0.43
1:C:538:LEU:HD12	1:A:348:ARG:CZ	2.48	0.43
1:D:377:ARG:NH2	1:D:426:ASP:OD2	2.52	0.43
1:D:447:SER:C	1:D:449:ARG:H	2.21	0.43
1:D:516:LYS:HG2	1:D:766:VAL:HG11	2.00	0.43
1:D:731:LEU:HD23	1:D:731:LEU:HA	1.82	0.43
1:A:377:ARG:NH2	1:A:426:ASP:OD2	2.51	0.43
1:B:88:ARG:HG2	1:B:335:PHE:HD1	1.84	0.43
1:C:478:ARG:NH1	1:C:566:PHE:CD2	2.87	0.43
1:C:687:LEU:HD23	1:C:687:LEU:HA	1.88	0.43
1:C:723:GLN:OE1	1:C:726:SER:HB2	2.18	0.43
1:E:97:GLY:HA2	1:E:318:GLU:OE1	2.19	0.43
1:F:315:ASP:OD1	1:F:359:LYS:N	2.44	0.43
1:F:628:TRP:HE1	1:F:646:THR:CG2	2.24	0.43
1:F:632:TRP:CE2	1:F:642:ILE:HD13	2.54	0.43
1:A:199:GLU:OE1	1:A:233:LYS:NZ	2.38	0.43
1:A:327:THR:HG1	1:A:379:TYR:HH	1.63	0.43
1:B:87:ILE:O	1:B:91:LEU:HD13	2.18	0.43
1:B:209:ALA:CA	1:B:214:LEU:HD21	2.48	0.43
1:C:285:PHE:HA	1:C:288:THR:O	2.19	0.43
1:E:545:PHE:HB3	1:E:593:ARG:NH1	2.34	0.43
1:D:223:LEU:O	1:D:227:TYR:HB2	2.19	0.43
1:F:270:LEU:HB2	1:F:360:ASN:CB	2.36	0.43
1:F:498:LYS:HB2	1:F:498:LYS:HE3	1.64	0.43
1:A:121:PRO:HB3	1:A:165:TRP:CZ2	2.54	0.43
1:A:128:ASP:O	1:A:132:GLN:HG3	2.19	0.43
1:A:181:GLU:O	1:A:184:TRP:HD1	2.01	0.43
1:B:144:SER:HB2	1:B:502:ARG:HH12	1.84	0.43
1:B:300:ILE:CG2	1:B:308:VAL:CG2	2.97	0.43
1:B:508:ASN:OD1	1:B:510:LEU:N	2.45	0.43
1:C:106:THR:HG21	1:C:129:TRP:CE3	2.54	0.43
1:E:352:PRO:O	1:E:387:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:ASP:OD2	1:D:313:PRO:HD3	2.19	0.43
1:D:329:LEU:HD12	1:D:484:TYR:HE2	1.83	0.43
1:D:373:PHE:CZ	1:D:385:PRO:HB3	2.53	0.43
1:D:657:PHE:O	1:D:659:GLY:N	2.50	0.43
1:D:676:LEU:HD13	1:D:736:PHE:CD2	2.54	0.43
1:F:477:PRO:HB2	1:F:566:PHE:HE2	1.84	0.43
1:A:297:LEU:O	1:A:301:VAL:HG23	2.19	0.43
1:A:558:TYR:CD1	1:A:558:TYR:C	2.92	0.43
1:A:692:LEU:O	1:A:696:ASN:HB2	2.18	0.43
1:B:638:SER:HB3	1:A:712:LEU:CD2	2.49	0.43
1:E:365:ASP:C	1:E:391:PHE:HE2	2.22	0.43
1:D:104:TYR:HB3	1:D:499:VAL:CG2	2.48	0.43
1:D:125:SER:HA	1:D:128:ASP:HB2	1.99	0.43
1:F:478:ARG:HA	1:F:478:ARG:HD2	1.43	0.43
1:F:577:TRP:HD1	1:F:577:TRP:O	2.02	0.43
1:A:226:ILE:HG21	1:A:226:ILE:HD13	1.76	0.43
1:A:242:LEU:HD22	1:A:243:HIS:CE1	2.54	0.43
1:A:375:LEU:HD23	1:A:375:LEU:HA	1.79	0.43
1:A:548:THR:O	1:A:550:PRO:HD3	2.18	0.43
1:A:613:PHE:HD1	1:A:614:ASP:N	2.17	0.43
1:B:325:ARG:HA	1:B:325:ARG:HD3	1.88	0.43
1:C:288:THR:HG22	1:C:290:ASP:HB2	2.01	0.43
1:C:452:ASP:HB3	1:C:455:ALA:O	2.19	0.43
1:C:589:SER:OG	1:C:592:ARG:NH2	2.45	0.43
1:E:576:GLY:HA3	1:E:657:PHE:CE2	2.54	0.43
1:E:605:GLU:O	1:E:608:ILE:HG22	2.19	0.43
1:D:325:ARG:HG3	1:D:506:PHE:CE1	2.54	0.43
1:F:264:LEU:HA	1:F:264:LEU:HD12	1.71	0.43
1:F:272:GLY:HA3	1:F:292:LYS:HG2	2.00	0.43
1:F:472:TRP:O	1:F:741:LYS:HE3	2.19	0.43
1:F:702:LYS:HA	1:F:702:LYS:HD3	1.82	0.43
1:A:265:LEU:HA	1:A:265:LEU:HD23	1.82	0.43
1:A:538:LEU:O	1:A:540:SER:N	2.51	0.43
1:B:529:GLU:HG2	1:B:558:TYR:OH	2.19	0.42
1:B:538:LEU:HD12	1:D:348:ARG:CZ	2.49	0.42
1:B:690:ARG:HD2	1:B:707:ASP:OD1	2.19	0.42
1:D:152:ILE:HG23	1:D:153:MET:N	2.33	0.42
1:D:403:GLU:HG2	1:D:405:ASN:ND2	2.34	0.42
1:D:660:ARG:HD2	1:D:729:ASN:ND2	2.34	0.42
1:F:319:ARG:CD	1:F:345:TYR:HD2	2.32	0.42
1:F:338:GLU:HA	1:F:341:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:561:ALA:O	1:F:565:ILE:HG23	2.19	0.42
1:F:687:LEU:HD13	1:F:710:VAL:HG21	2.00	0.42
1:A:157:ALA:HA	1:A:160:VAL:CG2	2.48	0.42
1:A:676:LEU:HD23	1:A:676:LEU:HA	1.65	0.42
1:A:699:SER:HB2	1:A:702:LYS:HB2	2.00	0.42
1:B:92:ARG:HH22	1:E:92:ARG:HH11	1.66	0.42
1:B:202:LEU:HD12	1:B:202:LEU:HA	1.80	0.42
1:B:300:ILE:HG23	1:B:308:VAL:HG23	2.00	0.42
1:C:131:VAL:HG23	1:C:162:LEU:HD21	2.01	0.42
1:C:291:GLN:O	1:C:295:GLU:HG3	2.19	0.42
1:C:670:LEU:HD23	1:C:670:LEU:C	2.40	0.42
1:E:676:LEU:HD23	1:E:676:LEU:HA	1.76	0.42
1:D:470:TYR:HE1	1:D:749:CYS:SG	2.41	0.42
1:D:728:ILE:O	1:D:729:ASN:C	2.57	0.42
1:F:84:ILE:HG23	1:F:335:PHE:CE1	2.53	0.42
1:F:202:LEU:O	1:F:206:LEU:HG	2.19	0.42
1:A:603:ASN:O	1:A:604:LEU:HB2	2.19	0.42
1:B:91:LEU:HD21	1:B:326:LEU:CD1	2.49	0.42
1:C:142:ASP:N	1:C:142:ASP:OD1	2.52	0.42
1:C:533:LEU:HD12	1:C:533:LEU:HA	1.62	0.42
1:C:691:VAL:O	1:C:695:GLU:HG2	2.19	0.42
1:F:126:THR:O	1:F:130:ILE:HG12	2.19	0.42
1:B:632:TRP:O	1:B:636:GLU:HB2	2.19	0.42
1:B:711:ASP:O	1:B:715:GLN:HG3	2.19	0.42
1:C:110:ALA:C	1:C:112:LEU:H	2.23	0.42
1:C:156:LEU:HD11	1:C:205:LEU:HG	2.00	0.42
1:C:173:GLU:HA	1:C:176:LEU:HB3	2.00	0.42
1:C:538:LEU:HD12	1:A:348:ARG:NH1	2.34	0.42
1:C:664:THR:CB	1:D:664:THR:H	2.32	0.42
1:E:408:SER:HB2	1:E:411:PRO:CD	2.49	0.42
1:F:276:CYS:O	1:F:311:ILE:HA	2.19	0.42
1:A:99:ILE:HG12	1:A:100:SER:N	2.34	0.42
1:A:153:MET:HE3	1:A:153:MET:HB2	1.66	0.42
1:A:419:SER:HB2	1:A:434:GLU:HB2	2.01	0.42
1:B:341:ASP:O	1:B:344:ASP:HB2	2.19	0.42
1:B:678:GLN:HG2	1:A:678:GLN:HG2	2.01	0.42
1:C:152:ILE:HG23	1:C:153:MET:H	1.85	0.42
1:C:233:LYS:HE3	1:C:233:LYS:HB3	1.84	0.42
1:E:549:ASP:HA	1:E:550:PRO:HD3	1.82	0.42
1:D:216:ILE:HA	1:D:217:PRO:HD3	1.85	0.42
1:D:420:GLN:HA	1:D:420:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:ILE:HD12	1:F:158:CYS:SG	2.60	0.42
1:A:94:ILE:HG23	1:A:319:ARG:NH2	2.34	0.42
1:B:102:SER:OG	1:B:105:ASP:HB2	2.20	0.42
1:B:444:ARG:HE	1:B:444:ARG:HB2	1.54	0.42
1:C:312:TYR:CG	1:C:313:PRO:HA	2.54	0.42
1:D:670:LEU:HD12	1:D:670:LEU:HA	1.85	0.42
1:F:721:VAL:HG11	1:F:737:LEU:HB2	2.02	0.42
1:F:745:TYR:CE1	1:F:749:CYS:SG	3.13	0.42
1:A:140:TRP:HD1	1:A:155:THR:HA	1.81	0.42
1:A:220:GLU:HB3	1:A:223:LEU:HD13	2.01	0.42
1:A:320:LEU:HD21	1:A:372:GLY:HA2	2.00	0.42
1:B:264:LEU:HD12	1:B:264:LEU:HA	1.73	0.42
1:C:163:LYS:HB2	1:C:163:LYS:HE2	1.73	0.42
1:C:300:ILE:HG21	1:C:308:VAL:HG23	2.01	0.42
1:C:543:GLU:C	1:C:545:PHE:H	2.21	0.42
1:C:632:TRP:CE2	1:C:642:ILE:HD13	2.54	0.42
1:E:412:MET:HG3	1:E:440:PHE:CD2	2.55	0.42
1:A:271:ASP:OD2	1:A:313:PRO:HD3	2.19	0.42
1:A:452:ASP:HB3	1:A:455:ALA:O	2.18	0.42
1:B:444:ARG:HG3	1:B:449:ARG:HB2	2.01	0.42
1:C:718:THR:O	1:C:722:LEU:HD13	2.20	0.42
1:D:96:GLU:HB2	1:D:303:LYS:HE3	2.00	0.42
1:D:427:ASP:OD1	1:D:428:GLY:N	2.53	0.42
1:D:444:ARG:HD2	1:D:449:ARG:HB2	2.01	0.42
1:F:135:LEU:CD1	1:F:137:ASP:HB3	2.48	0.42
1:A:83:MET:HE3	1:A:514:ALA:HA	2.02	0.42
1:A:546:GLY:HA3	1:A:550:PRO:HG3	2.01	0.42
1:B:130:ILE:O	1:B:140:TRP:CZ3	2.73	0.42
1:B:479:ILE:HD11	1:B:559:PHE:HZ	1.84	0.42
1:E:377:ARG:HD3	1:E:421:LEU:CB	2.50	0.42
1:D:320:LEU:HD21	1:D:372:GLY:HA2	2.01	0.42
1:D:341:ASP:O	1:D:344:ASP:HB2	2.19	0.42
1:F:321:TRP:CZ3	1:F:325:ARG:NH2	2.88	0.42
1:F:366:ILE:HA	1:F:391:PHE:HE2	1.85	0.42
1:F:473:LYS:O	1:F:741:LYS:HG2	2.20	0.42
1:F:482:ARG:NH2	1:F:766:VAL:HG13	2.34	0.42
1:A:96:GLU:HB3	1:A:312:TYR:CE2	2.55	0.42
1:A:461:PRO:O	1:A:465:GLU:N	2.45	0.42
1:A:466:TYR:CE1	1:A:470:TYR:HB2	2.55	0.42
1:A:662:VAL:O	1:A:662:VAL:HG23	2.19	0.42
1:A:687:LEU:O	1:A:691:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:LEU:HD22	1:B:168:HIS:HB2	2.02	0.42
1:B:300:ILE:HG21	1:B:308:VAL:CG2	2.50	0.42
1:C:304:PHE:CE2	1:C:309:PRO:HD3	2.55	0.42
1:E:142:ASP:OD1	1:E:502:ARG:NH1	2.52	0.42
1:E:193:TRP:CH2	1:E:451:LYS:HD3	2.53	0.42
1:E:545:PHE:HB3	1:E:593:ARG:CZ	2.49	0.42
1:D:91:LEU:HD23	1:D:91:LEU:HA	1.58	0.42
1:B:300:ILE:CG2	1:B:308:VAL:HG23	2.50	0.41
1:B:412:MET:HA	1:B:415:THR:OG1	2.20	0.41
1:B:559:PHE:CG	1:B:758:ILE:HG12	2.55	0.41
1:C:664:THR:HG1	1:C:665:GLY:H	1.62	0.41
1:C:675:GLN:HG2	1:C:720:ARG:CZ	2.50	0.41
1:D:556:THR:HG22	1:D:758:ILE:HD11	2.02	0.41
1:D:755:ASP:HB3	1:D:758:ILE:HD12	2.02	0.41
1:F:135:LEU:HB2	1:F:136:PRO:HD2	2.01	0.41
1:C:513:LYS:HD3	1:C:513:LYS:HA	1.90	0.41
1:E:671:TRP:HH2	1:F:656:ILE:HD11	1.85	0.41
1:D:104:TYR:HD2	1:D:153:MET:HG2	1.81	0.41
1:D:458:LYS:HE2	1:D:486:ASP:O	2.20	0.41
1:F:376:LEU:HD23	1:F:376:LEU:HA	1.85	0.41
1:F:529:GLU:HG2	1:F:558:TYR:OH	2.20	0.41
1:A:153:MET:HE2	1:A:202:LEU:HD13	2.03	0.41
1:A:690:ARG:HG3	1:A:691:VAL:N	2.35	0.41
1:B:690:ARG:HB2	1:B:706:ILE:HG21	2.02	0.41
1:B:766:VAL:O	1:B:767:ILE:HG22	2.20	0.41
1:C:348:ARG:HG2	1:C:348:ARG:HH11	1.85	0.41
1:C:482:ARG:HG2	1:C:761:VAL:HA	2.01	0.41
1:C:692:LEU:HA	1:C:695:GLU:HG3	2.01	0.41
1:E:444:ARG:HE	1:E:444:ARG:HB2	1.35	0.41
1:D:135:LEU:HD11	1:D:139:SER:HB2	2.02	0.41
1:D:224:LYS:HB3	1:D:224:LYS:HE3	1.87	0.41
1:D:291:GLN:O	1:D:295:GLU:HG3	2.21	0.41
1:A:281:THR:HB	1:A:297:LEU:HD21	2.01	0.41
1:A:754:ILE:O	1:A:758:ILE:HG13	2.20	0.41
1:C:320:LEU:CD2	1:C:372:GLY:HA2	2.49	0.41
1:D:377:ARG:HD3	1:D:421:LEU:HB3	2.02	0.41
1:F:470:TYR:N	1:F:470:TYR:CD1	2.89	0.41
1:F:731:LEU:HD23	1:F:731:LEU:HA	1.71	0.41
1:A:133:ASN:OD1	1:A:133:ASN:N	2.52	0.41
1:A:478:ARG:HD2	1:A:478:ARG:HA	1.52	0.41
1:D:173:GLU:O	1:D:175:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:MET:HG3	1:D:198:PHE:CD2	2.47	0.41
1:D:403:GLU:HG2	1:D:405:ASN:HD21	1.84	0.41
1:F:80:THR:HG23	1:F:517:ALA:HB1	2.02	0.41
1:F:392:GLU:HB2	1:F:397:PHE:CE1	2.56	0.41
1:F:456:ILE:HD12	1:F:456:ILE:HA	1.93	0.41
1:A:135:LEU:HD11	1:A:143:ALA:HB2	2.01	0.41
1:A:621:LEU:HD12	1:A:621:LEU:HA	1.83	0.41
1:E:375:LEU:HD23	1:E:375:LEU:HA	1.83	0.41
1:E:385:PRO:CB	1:E:430:LEU:HD13	2.50	0.41
1:F:263:LYS:HE2	1:F:263:LYS:HB3	1.64	0.41
1:F:514:ALA:O	1:F:517:ALA:HB3	2.20	0.41
1:B:268:ARG:HH11	1:B:293:CYS:HB2	1.85	0.41
1:B:285:PHE:HA	1:B:288:THR:O	2.21	0.41
1:B:478:ARG:HD2	1:B:478:ARG:HA	1.72	0.41
1:C:331:ILE:HG21	1:C:331:ILE:HD13	1.83	0.41
1:E:328:ARG:HB3	1:E:484:TYR:CD2	2.55	0.41
1:E:614:ASP:HB3	1:E:617:TYR:HB2	2.01	0.41
1:D:325:ARG:CG	1:D:506:PHE:CE1	3.03	0.41
1:D:377:ARG:NH1	1:D:383:VAL:HG23	2.35	0.41
1:D:445:ARG:HH11	1:D:465:GLU:HG3	1.85	0.41
1:D:472:TRP:O	1:D:741:LYS:HE3	2.20	0.41
1:C:196:VAL:HG22	1:C:497:GLY:O	2.20	0.41
1:C:730:ARG:O	1:C:734:GLU:HG3	2.20	0.41
1:D:321:TRP:HZ3	1:D:325:ARG:NH2	2.18	0.41
1:D:664:THR:HG23	1:D:670:LEU:HD13	2.02	0.41
1:A:169:THR:HA	1:A:172:CYS:CB	2.49	0.41
1:C:223:LEU:O	1:C:225:ALA:N	2.53	0.41
1:C:352:PRO:O	1:C:387:VAL:HG23	2.20	0.41
1:C:377:ARG:HD3	1:C:421:LEU:HB3	2.02	0.41
1:C:423:PHE:CZ	1:C:719:ARG:HA	2.56	0.41
1:E:329:LEU:HA	1:E:329:LEU:HD23	1.87	0.41
1:E:419:SER:HA	1:E:430:LEU:HG	2.02	0.41
1:E:478:ARG:HD2	1:E:478:ARG:HA	1.58	0.41
1:E:533:LEU:HD22	1:E:554:LEU:HD11	2.02	0.41
1:D:292:LYS:HA	1:D:292:LYS:HD2	1.83	0.41
1:D:297:LEU:HD23	1:D:297:LEU:HA	1.78	0.41
1:D:535:ARG:HG2	1:D:539:ARG:HD3	2.02	0.41
1:F:262:GLU:HG2	1:F:263:LYS:N	2.36	0.41
1:F:313:PRO:HG2	1:F:358:THR:OG1	2.21	0.41
1:F:754:ILE:O	1:F:758:ILE:HG13	2.21	0.41
1:A:206:LEU:HD23	1:A:210:LYS:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:VAL:HG12	1:A:432:ARG:HH12	1.85	0.41
1:A:628:TRP:HE1	1:A:646:THR:HG23	1.85	0.41
1:B:320:LEU:HD23	1:B:320:LEU:HA	1.89	0.41
1:B:489:GLY:HA3	1:B:493:ASP:OD1	2.21	0.41
1:B:542:LEU:HD12	1:B:542:LEU:HA	1.84	0.41
1:C:714:MET:HE2	1:C:714:MET:HB2	1.96	0.41
1:E:320:LEU:HA	1:E:320:LEU:HD23	1.85	0.41
1:E:344:ASP:HB3	1:E:348:ARG:HH22	1.85	0.41
1:D:335:PHE:HB3	1:D:338:GLU:CG	2.51	0.41
1:A:83:MET:HG2	1:A:510:LEU:HD11	2.03	0.41
1:A:168:HIS:O	1:A:172:CYS:HB2	2.21	0.41
1:A:292:LYS:H	1:A:292:LYS:HG2	1.56	0.41
1:A:494:VAL:HG22	1:A:502:ARG:NH2	2.36	0.41
1:B:535:ARG:NH1	1:D:340:GLU:OE1	2.51	0.40
1:E:540:SER:O	1:E:542:LEU:HD12	2.21	0.40
1:D:187:ALA:HB2	1:D:222:ALA:HB2	2.02	0.40
1:D:676:LEU:HA	1:D:676:LEU:HD23	1.69	0.40
1:F:343:LEU:HD23	1:F:346:ILE:HG13	2.03	0.40
1:F:676:LEU:HA	1:F:676:LEU:HD23	1.75	0.40
1:A:302:LYS:HG3	1:A:303:LYS:H	1.85	0.40
1:A:346:ILE:HG22	1:A:376:LEU:HD11	2.02	0.40
1:A:374:ARG:HB2	1:A:418:ALA:HB2	2.04	0.40
1:B:88:ARG:HG2	1:B:335:PHE:CE1	2.56	0.40
1:B:140:TRP:CD1	1:B:155:THR:HA	2.57	0.40
1:B:720:ARG:HH12	1:A:627:GLN:CD	2.24	0.40
1:C:422:LYS:H	1:C:422:LYS:HG2	1.64	0.40
1:C:678:GLN:HG2	1:D:678:GLN:HG2	2.04	0.40
1:E:131:VAL:HG23	1:E:132:GLN:HG3	2.02	0.40
1:E:297:LEU:HD23	1:E:297:LEU:HA	1.75	0.40
1:F:343:LEU:HD23	1:F:343:LEU:HA	1.61	0.40
1:A:165:TRP:O	1:A:167:ILE:HG23	2.21	0.40
1:A:206:LEU:HD11	1:A:218:TYR:HB3	2.02	0.40
1:A:312:TYR:CD2	1:A:313:PRO:HA	2.56	0.40
1:A:613:PHE:CE1	1:A:617:TYR:CD2	3.09	0.40
1:B:173:GLU:HA	1:B:176:LEU:HB3	2.03	0.40
1:B:195:LEU:HD11	1:B:498:LYS:O	2.20	0.40
1:B:495:TRP:CD1	1:B:503:MET:HG2	2.57	0.40
1:B:566:PHE:CD1	1:B:566:PHE:N	2.87	0.40
1:C:156:LEU:HD11	1:C:205:LEU:HD21	2.03	0.40
1:C:325:ARG:HA	1:C:325:ARG:HD3	1.70	0.40
1:E:412:MET:HB2	1:E:441:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:687:LEU:HD23	1:E:687:LEU:HA	1.92	0.40
1:D:97:GLY:HA2	1:D:318:GLU:OE1	2.21	0.40
1:D:728:ILE:HG21	1:D:728:ILE:HD13	1.85	0.40
1:F:755:ASP:HA	1:F:758:ILE:HB	2.03	0.40
1:A:105:ASP:OD2	1:A:278:PRO:HD2	2.22	0.40
1:B:376:LEU:HD23	1:B:376:LEU:HA	1.71	0.40
1:B:423:PHE:CE1	1:B:719:ARG:HA	2.56	0.40
1:B:650:LEU:HA	1:B:650:LEU:HD23	1.87	0.40
1:C:482:ARG:HB2	1:C:519:PHE:CZ	2.56	0.40
1:E:190:GLU:HG3	1:E:193:TRP:CE3	2.54	0.40
1:E:650:LEU:HD23	1:E:650:LEU:HA	1.59	0.40
1:D:312:TYR:CG	1:D:313:PRO:HA	2.56	0.40
1:D:664:THR:CG2	1:D:670:LEU:HD13	2.51	0.40
1:F:422:LYS:HB3	1:F:422:LYS:HE2	1.76	0.40
1:F:683:ILE:O	1:F:687:LEU:HB2	2.20	0.40
1:A:162:LEU:HA	1:A:162:LEU:HD23	1.81	0.40
1:A:445:ARG:HA	1:A:450:MET:CE	2.52	0.40
1:A:574:ARG:O	1:A:577:TRP:HB3	2.22	0.40
1:A:642:ILE:H	1:A:642:ILE:HG13	1.81	0.40
1:B:206:LEU:HD11	1:B:223:LEU:HD21	2.02	0.40
1:B:321:TRP:O	1:B:325:ARG:HG2	2.22	0.40
1:B:389:LYS:HB3	1:B:429:VAL:CG1	2.49	0.40
1:B:698:GLU:O	1:B:699:SER:HB2	2.22	0.40
1:C:239:ARG:HA	1:C:239:ARG:HD3	1.78	0.40
1:C:508:ASN:OD1	1:C:509:ASP:N	2.55	0.40
1:D:321:TRP:CZ3	1:D:325:ARG:NH2	2.90	0.40
1:D:484:TYR:HA	1:D:487:GLN:HG3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	687/775 (89%)	621 (90%)	56 (8%)	10 (2%)	10	45
1	B	658/775 (85%)	611 (93%)	37 (6%)	10 (2%)	10	45
1	C	635/775 (82%)	571 (90%)	52 (8%)	12 (2%)	8	40
1	D	686/775 (88%)	637 (93%)	41 (6%)	8 (1%)	13	50
1	E	686/775 (88%)	630 (92%)	49 (7%)	7 (1%)	15	54
1	F	671/775 (87%)	605 (90%)	57 (8%)	9 (1%)	12	48
All	All	4023/4650 (86%)	3675 (91%)	292 (7%)	56 (1%)	11	46

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	403	GLU
1	B	607	LEU
1	B	697	GLY
1	C	183	MET
1	C	664	THR
1	C	697	GLY
1	F	218	TYR
1	F	258	ASP
1	A	99	ILE
1	A	694	GLN
1	A	698	GLU
1	B	606	GLU
1	B	723	GLN
1	C	174	ARG
1	C	224	LYS
1	C	723	GLN
1	E	548	THR
1	E	697	GLY
1	D	174	ARG
1	D	658	GLY
1	D	699	SER
1	F	117	GLY
1	F	174	ARG
1	F	404	SER
1	F	663	LEU
1	F	724	GLY
1	A	394	ASP
1	A	696	ASN
1	B	539	ARG
1	B	594	ILE

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Mol	Chain	Res	Type
1	B	699	SER
1	A	191	GLU
1	A	213	ASP
1	A	238	PRO
1	B	458	LYS
1	C	725	CYS
1	E	230	ARG
1	E	699	SER
1	D	548	THR
1	A	450	MET
1	B	217	PRO
1	C	699	SER
1	E	696	ASN
1	D	111	LEU
1	F	402	GLY
1	C	125	SER
1	C	550	PRO
1	E	111	LEU
1	D	175	GLY
1	D	663	LEU
1	A	699	SER
1	E	118	GLY
1	D	406	PRO
1	C	175	GLY
1	F	175	GLY
1	C	138	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	598/672 (89%)	571 (96%)	27 (4%)	27	61
1	B	582/672 (87%)	563 (97%)	19 (3%)	38	68
1	C	565/672 (84%)	547 (97%)	18 (3%)	39	69
1	D	597/672 (89%)	580 (97%)	17 (3%)	43	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	597/672 (89%)	568 (95%)	29 (5%)	25	59
1	F	589/672 (88%)	569 (97%)	20 (3%)	37	68
All	All	3528/4032 (88%)	3398 (96%)	130 (4%)	34	65

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	102	SER
1	B	164	SER
1	B	165	TRP
1	B	213	ASP
1	B	214	LEU
1	B	227	TYR
1	B	263	LYS
1	B	314	LEU
1	B	315	ASP
1	B	333	ARG
1	B	420	GLN
1	B	444	ARG
1	B	478	ARG
1	B	529	GLU
1	B	537	TYR
1	B	604	LEU
1	B	618	SER
1	B	711	ASP
1	B	726	SER
1	C	146	PHE
1	C	193	TRP
1	C	204	SER
1	C	232	ARG
1	C	259	LEU
1	C	271	ASP
1	C	277	SER
1	C	360	ASN
1	C	478	ARG
1	C	506	PHE
1	C	512	LEU
1	C	537	TYR
1	C	545	PHE
1	C	591	PHE
1	C	599	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	641	SER
1	C	690	ARG
1	C	711	ASP
1	E	102	SER
1	E	114	ARG
1	E	119	ASP
1	E	145	PHE
1	E	170	ASP
1	E	210	LYS
1	E	219	ASP
1	E	220	GLU
1	E	227	TYR
1	E	230	ARG
1	E	232	ARG
1	E	239	ARG
1	E	261	TRP
1	E	315	ASP
1	E	333	ARG
1	E	360	ASN
1	E	440	PHE
1	E	444	ARG
1	E	453	LYS
1	E	478	ARG
1	E	512	LEU
1	E	541	ASN
1	E	545	PHE
1	E	549	ASP
1	E	592	ARG
1	E	599	ASN
1	E	615	ASP
1	E	641	SER
1	E	643	GLU
1	D	102	SER
1	D	116	ASP
1	D	144	SER
1	D	190	GLU
1	D	227	TYR
1	D	239	ARG
1	D	259	LEU
1	D	315	ASP
1	D	478	ARG
1	D	487	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	506	PHE
1	D	512	LEU
1	D	537	TYR
1	D	545	PHE
1	D	604	LEU
1	D	690	ARG
1	D	730	ARG
1	F	165	TRP
1	F	166	ASN
1	F	220	GLU
1	F	227	TYR
1	F	256	MET
1	F	271	ASP
1	F	277	SER
1	F	287	GLN
1	F	317	TYR
1	F	360	ASN
1	F	394	ASP
1	F	417	ARG
1	F	445	ARG
1	F	468	MET
1	F	613	PHE
1	F	618	SER
1	F	622	ARG
1	F	666	GLN
1	F	726	SER
1	F	730	ARG
1	A	133	ASN
1	A	192	ASP
1	A	193	TRP
1	A	227	TYR
1	A	239	ARG
1	A	245	MET
1	A	259	LEU
1	A	280	SER
1	A	291	GLN
1	A	293	CYS
1	A	305	ASN
1	A	337	SER
1	A	444	ARG
1	A	447	SER
1	A	478	ARG

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Mol	Chain	Res	Type
1	A	539	ARG
1	A	545	PHE
1	A	549	ASP
1	A	569	ASN
1	A	591	PHE
1	A	599	ASN
1	A	609	SER
1	A	613	PHE
1	A	622	ARG
1	A	632	TRP
1	A	690	ARG
1	A	723	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	420	GLN
1	C	251	HIS
1	E	420	GLN
1	D	420	GLN
1	F	420	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	689/775 (88%)	0.33	3 (0%) 92   90	32, 56, 100, 127	0
1	B	668/775 (86%)	0.56	39 (5%) 23   20	34, 76, 118, 132	0
1	C	648/775 (83%)	0.72	69 (10%) 6   7	39, 85, 150, 177	0
1	D	688/775 (88%)	0.67	65 (9%) 8   9	41, 84, 138, 160	0
1	E	688/775 (88%)	0.31	3 (0%) 92   90	41, 67, 111, 131	0
1	F	677/775 (87%)	0.75	68 (10%) 7   8	50, 95, 145, 169	0
All	All	4058/4650 (87%)	0.55	247 (6%) 21   19	32, 76, 135, 177	0

All (247) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	496	ILE	5.6
1	D	454	TRP	5.2
1	F	192	ASP	5.1
1	C	200	ILE	5.1
1	C	104	TYR	4.6
1	C	179	ILE	4.6
1	C	497	GLY	4.6
1	C	105	ASP	4.5
1	C	180	GLN	4.2
1	D	160	VAL	4.2
1	F	454	TRP	4.0
1	C	159	VAL	3.9
1	C	357	HIS	3.9
1	F	193	TRP	3.8
1	F	176	LEU	3.8
1	C	106	THR	3.8
1	F	500	LEU	3.7
1	D	127	ILE	3.7
1	C	112	LEU	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	243	HIS	3.6
1	F	179	ILE	3.6
1	D	221	PRO	3.6
1	C	155	THR	3.6
1	B	498	LYS	3.6
1	C	300	ILE	3.6
1	C	152	ILE	3.5
1	C	500	LEU	3.4
1	C	454	TRP	3.4
1	D	253	LEU	3.4
1	F	617	TYR	3.3
1	B	256	MET	3.3
1	C	253	LEU	3.3
1	B	216	ILE	3.3
1	C	256	MET	3.3
1	C	296	TYR	3.2
1	D	104	TYR	3.2
1	F	172	CYS	3.2
1	C	111	LEU	3.2
1	D	261	TRP	3.2
1	D	107	SER	3.2
1	C	279	ALA	3.2
1	D	108	LEU	3.2
1	F	138	GLY	3.2
1	D	126	THR	3.1
1	C	278	PRO	3.1
1	D	208	MET	3.1
1	D	252	SER	3.1
1	C	314	LEU	3.1
1	C	313	PRO	3.0
1	D	222	ALA	3.0
1	F	307	GLY	3.0
1	D	180	GLN	3.0
1	B	198	PHE	3.0
1	C	252	SER	3.0
1	D	307	GLY	3.0
1	D	109	VAL	3.0
1	D	159	VAL	3.0
1	D	141	GLY	3.0
1	F	157	ALA	3.0
1	C	251	HIS	3.0
1	C	131	VAL	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	104	TYR	2.9
1	D	297	LEU	2.9
1	F	450	MET	2.9
1	C	165	TRP	2.9
1	C	153	MET	2.9
1	C	99	ILE	2.9
1	F	314	LEU	2.9
1	F	761	VAL	2.8
1	D	495	TRP	2.8
1	C	504	THR	2.8
1	C	156	LEU	2.8
1	D	200	ILE	2.8
1	D	182	ASN	2.8
1	C	108	LEU	2.8
1	F	103	ALA	2.8
1	D	400	LEU	2.8
1	B	251	HIS	2.8
1	C	148	MET	2.7
1	C	311	ILE	2.7
1	C	485	LEU	2.7
1	D	455	ALA	2.7
1	B	286	GLN	2.7
1	C	371	MET	2.7
1	F	153	MET	2.7
1	C	181	GLU	2.7
1	F	563	ALA	2.7
1	F	91	LEU	2.7
1	B	148	MET	2.7
1	C	309	PRO	2.7
1	D	453	LYS	2.7
1	B	215	ASP	2.7
1	B	156	LEU	2.7
1	D	157	ALA	2.7
1	D	215	ASP	2.6
1	D	238	PRO	2.6
1	F	616	ALA	2.6
1	D	165	TRP	2.6
1	F	308	VAL	2.6
1	F	99	ILE	2.6
1	A	239	ARG	2.6
1	C	283	THR	2.6
1	B	500	LEU	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	103	ALA	2.6
1	D	496	ILE	2.6
1	C	205	LEU	2.6
1	F	420	GLN	2.6
1	F	506	PHE	2.6
1	F	178	PHE	2.6
1	F	398	PHE	2.6
1	B	311	ILE	2.6
1	F	300	ILE	2.6
1	D	460	ILE	2.6
1	F	123	PHE	2.5
1	B	217	PRO	2.5
1	C	127	ILE	2.5
1	D	174	ARG	2.5
1	C	400	LEU	2.5
1	C	310	CYS	2.5
1	F	183	MET	2.5
1	B	280	SER	2.5
1	D	179	ILE	2.5
1	C	174	ARG	2.5
1	C	162	LEU	2.5
1	D	278	PRO	2.5
1	D	309	PRO	2.5
1	C	505	LEU	2.5
1	C	498	LYS	2.5
1	F	503	MET	2.5
1	D	146	PHE	2.5
1	F	317	TYR	2.5
1	F	498	LYS	2.5
1	D	131	VAL	2.4
1	F	108	LEU	2.4
1	B	178	PHE	2.4
1	B	318	GLU	2.4
1	D	300	ILE	2.4
1	B	205	LEU	2.4
1	F	400	LEU	2.4
1	D	254	GLU	2.4
1	C	208	MET	2.4
1	C	318	GLU	2.4
1	F	309	PRO	2.4
1	D	321	TRP	2.4
1	D	398	PHE	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	149	GLY	2.4
1	B	397	PHE	2.4
1	D	103	ALA	2.4
1	F	184	TRP	2.4
1	B	180	GLN	2.4
1	B	485	LEU	2.4
1	C	317	TYR	2.4
1	F	502	ARG	2.4
1	F	222	ALA	2.4
1	F	762	ILE	2.4
1	C	399	CYS	2.4
1	B	516	LYS	2.4
1	B	208	MET	2.4
1	D	274	PHE	2.4
1	F	186	LEU	2.4
1	D	225	ALA	2.3
1	D	161	ALA	2.3
1	F	412	MET	2.3
1	F	764	GLN	2.3
1	C	274	PHE	2.3
1	F	111	LEU	2.3
1	A	274	PHE	2.3
1	B	261	TRP	2.3
1	F	401	HIS	2.3
1	B	300	ILE	2.3
1	C	150	ASP	2.3
1	B	297	LEU	2.3
1	F	451	LYS	2.3
1	B	252	SER	2.3
1	F	214	LEU	2.3
1	D	357	HIS	2.3
1	F	104	TYR	2.3
1	D	149	GLY	2.3
1	B	279	ALA	2.3
1	C	282	ALA	2.3
1	B	153	MET	2.2
1	F	215	ASP	2.2
1	D	99	ILE	2.2
1	E	283	THR	2.2
1	B	488	TYR	2.2
1	C	280	SER	2.2
1	C	506	PHE	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	762	ILE	2.2
1	F	143	ALA	2.2
1	C	161	ALA	2.2
1	D	153	MET	2.2
1	C	178	PHE	2.2
1	F	281	THR	2.2
1	C	242	LEU	2.2
1	C	197	GLY	2.2
1	B	309	PRO	2.2
1	F	109	VAL	2.2
1	B	199	GLU	2.2
1	B	141	GLY	2.2
1	F	593	ARG	2.2
1	D	317	TYR	2.1
1	D	156	LEU	2.1
1	D	178	PHE	2.1
1	F	113	LYS	2.1
1	C	271	ASP	2.1
1	F	320	LEU	2.1
1	B	242	LEU	2.1
1	C	261	TRP	2.1
1	C	281	THR	2.1
1	D	293	CYS	2.1
1	A	99	ILE	2.1
1	F	142	ASP	2.1
1	E	698	GLU	2.1
1	F	246	PRO	2.1
1	B	254	GLU	2.1
1	F	365	ASP	2.1
1	B	314	LEU	2.1
1	D	500	LEU	2.1
1	F	149	GLY	2.1
1	C	262	GLU	2.1
1	D	331	ILE	2.1
1	F	329	LEU	2.1
1	F	397	PHE	2.1
1	D	173	GLU	2.1
1	D	498	LYS	2.1
1	F	311	ILE	2.1
1	F	106	THR	2.1
1	D	313	PRO	2.1
1	F	316	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	142	ASP	2.1
1	B	157	ALA	2.0
1	D	452	ASP	2.0
1	D	111	LEU	2.0
1	B	450	MET	2.0
1	F	452	ASP	2.0
1	C	397	PHE	2.0
1	D	281	THR	2.0
1	E	213	ASP	2.0
1	F	518	ASP	2.0
1	F	180	GLN	2.0
1	F	199	GLU	2.0
1	F	318	GLU	2.0
1	D	408	SER	2.0
1	B	103	ALA	2.0
1	B	179	ILE	2.0
1	F	463	GLU	2.0
1	D	195	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.